

- **SANS Data Reduction Tutorial**

10/2003 Version 4.2

This tutorial guides you through the basic features of data reduction using IGOR Pro.

For a "hands-on" experience, you may download the set of Tutorial Data, or use your own data, although there are some specific references to the Tutorial set. To work through the tutorial on your own, you must already have IGOR Pro and the SANS Reduction procedures installed. Once installed, open a blank data reduction experiment "SANS_Reduction.pxt", or a similar version. In addition to this help file, all SANS panels include balloon help (Mac) or command-line help (PC) that describes the action of each button or field in a panel.

General Description

[SANS Overview](#)

[Data Reduction Overview](#)

[What's New in SANS](#)

[Instructions for the Impatient](#)

Tutorial Instructions

[Main Controls](#)

[List the Data Files](#)

[The Display Window](#)

[Average Options](#)

[Calculate Transmissions](#)

[Patch File Headers](#)

[Build a Data Reduction Protocol](#)

[Reduce a File](#)

[Schematic of Data Reduction Operation](#)

[Reduce Multiple Files](#)

[Plot Averaged Data](#)

[Sort and Combine Averaged Datasets](#)

Additional Operations

[Main Panel Tabs](#)

[Fit Lines to Your Data](#)

[Subtract 1D Data](#)

[Draw a Mask](#)

[Marquee Operations](#)

[Tile 2-D Images](#)

[2-D ASCII Export](#)
[Copy Work Folder Contents](#)
[2-D Work File Arithmetic](#)
[SANS Preferences](#)
[3-D Display](#)
[Detector Sensitivity File](#)
[Real Time Data Display](#)

General Description

SANS Overview

The SANS Data Reduction using IGOR Pro is an implementation of the VAX data reduction procedures in an easier to use, graphical interface. It is designed to work on Macintosh or PC, and works directly on raw binary data files as collected on the VAX. All Raw SANS data files and reduction software can be carried to your home institution.

The procedures and software that are available for displaying and processing 2D SANS data (subtracting background, converting to an absolute scale, averaging, etc.) to produce reduced 1D or 2D data in intensity versus wavenumber (I vs. Q) form are described in the following sections. This section describes the underlying concepts of data reduction and the organization of the reduction program.

The raw, 2D (128 rows x 128 columns) data collected at the instruments resides in SANS user accounts in the form of individually named binary files. The format of the data file names is:

XXXXXNNN.SAn_INI_AMMM

where **XXXXX** is a 5-character sample prefix, **NNN** is an automatically incremented 3-digit run number, and **SAn** denotes the SANS instrument where the data was collected (**n**=1 for the NG1 SANS instrument, **n**=3 for NG3, and **n**=2 for NG7 SANS). **INI** denotes the user's initials, and **AMMM** is a 4-digit alphanumeric run identifier for archiving purposes. Raw data files are stored on the VAX and are protected from deletion. In addition, during your SANS experiment, as each data file is collected on the VAX, the raw data files are mirrored to a central server, "Charlotte". If your SANS account is NG3SANS41, your data will be located in the "NG3SANS41" folder on Charlotte. Charlotte is visible to Macs through Appleshare (connect as a guest), and to Windows through the Network Neighborhood (NCNR group, Map the "SANS Data" folder as a network drive). This central server allows you to (within the building) work directly with the data on Charlotte. The data on the VAX remains untouched, as a backup. You can see and reduce the data while at the instrument, in the computer room, or in the user offices. Once your experiment is finished, all of your data - raw data files, averaged data, IGOR Demo version (if needed), SANS Reduction Macros... can be copied from Charlotte onto a Zip disk or CD and carried home (a typical SANS session will produce between 2-6 MB of raw data). Data reduction can be completed (if necessary) at your home institution, without having to work around the NIST Firewall. FTP'ing of raw binary data from the NCNR to your home institution is not recommended, as the binary data structure is not always preserved even in a "binary" transfer.

The 128x128 data values in the raw data files are never altered; only the file header, which contains parameters such as the beam center coordinates, transmission, detector distance, etc. can be modified (using a Patch operation). For analysis, the data are loaded into a working folder "EXT", where EXT is a 3-letter mnemonic of the data "type" that represents the logical function of the data in the reduction sequence or the result of a processing step. For example, **SAM**, **EMP**, and **BGD** represent sample data, empy cell data, and background data, respectively. The data type **COR** identifies the results of combining the **SAM**, **EMP**, and **BGD** data to produce sample data that has been corrected for background and empty cell scattering.

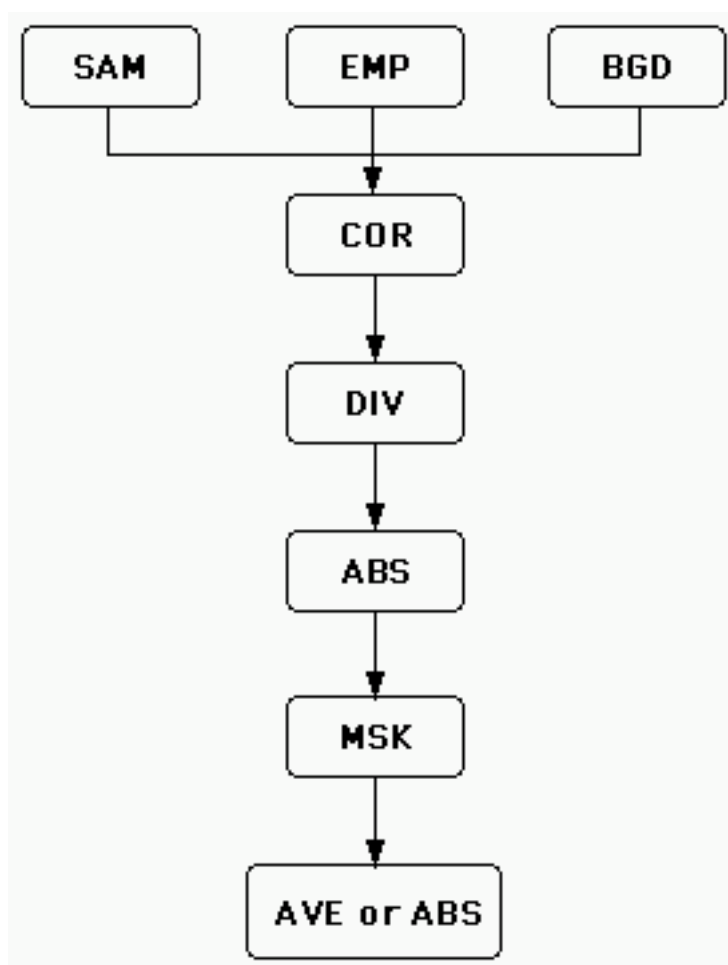
The data in work folders are processed by invoking a protocol that performs a sequence of specific operations, in some cases writing the result to a different work folder, overwriting the previous contents. Ultimately, the corrected data is saved to disk in the desired format in an "averaging" step. Typically the 2D data is circularly averaged to produce 1D (I vs. Q) ASCII data files. These 1D data files contain instrumental resolution information in addition to the intensity data. The "averaging" step can be configured to save a variety of 1D formats, including 2D ASCII files or PNG graphics images. See [Average Options](#) for details.

Once data are reduced to I vs. Q form, various types of linearized fits can be performed. See [Fit Lines to Your Data](#) for details.

Data Reduction Overview

Many of the data reduction programs make use of information recorded in the raw data header at the time the data were taken. Therefore, the correct values of parameters such as the X-Y coordinates of the beam center, the detector offset, the sample transmission, etc. must be in the raw data header before proceeding with the data reduction. Parameter values can be viewed and edited using the [Patch File Headers](#) operation which operates on one file at a time, or can operate on multiple files. Only the raw data headers are modified, leaving the data unaffected. Be sure to patch file headers with the correct values before proceeding with data correction.

The most commonly used sequence (or protocol) of data reduction steps is shown schematically in the figure below.



Initial correction

As data is loaded for use as SAM, EMP or BGD data types, each dataset is normalized to a fixed number of incident neutrons (corresponding to a monitor count of 10^8 counts) to facilitate comparisons between data sets. Sample data is corrected for background and empty cell scattering according to the algorithm:

$$\text{COR} = (\text{SAM} - \text{BGD}) - [\text{Tsam}/\text{Temp}](\text{EMP} - \text{BGD})$$

where Tsam is the transmission of the sample and Temp is that of the empty cell. Note that Tsam and Temp are taken with respect to the empty beam. Thus, if no cell is used (i.e., empty beam condition), Temp = 1.0. The results of this operation are stored in another work folder, COR.

Detector Efficiency Corrections

An important step in the data reduction process involves correcting for the detector response. A data set can be corrected for non-uniformities in the detector efficiency by dividing the data, pixel-by-pixel, by the measured scattering from an isotropic scatterer such as plexiglass or water. Plexiglass runs are measured periodically by the instrument scientists for this purpose and saved as **PLEX_DDMMYY_NGn.DIV** files which indicate the date the measurement was made (DDMMYY) and the instrument used (NGn). These files are stored on Charlotte in a folder named **NGn_FILES**. The DIV file for the current

cycle should be copied to your directory before reducing your data.

Subsequently the corrected data, COR, is divided, pixel-by-pixel, by the contents of DIV. This calibrated result is written to a separate work folder, CAL.

Absolute Scaling (optional)

At this point the CAL data may be converted to an absolute intensity scale ($I(Q) \rightarrow d\sigma(Q)/d\Omega$ in units of cm^{-1}) by specifying an absolute scaling factor. In order to find the scaling factor, the scattering from a standard sample or an attenuated empty beam must have been measured under the same experimental conditions. The scattered intensity $I(Q)$ produced by the averaging operation is related to the absolute cross-section $d\sigma(Q)/d\Omega$ by the expression:

$$I(Q) = \Phi A d T (d\sigma(Q)/d\Omega) \Delta\Omega \epsilon t,$$

where:

Φ = flux on the sample,

A = sample area,

d = sample thickness,

T = measured sample transmission,

$\Delta\Omega$ = solid angle subtended by one pixel of the detector,

ϵ = detector efficiency, and

t = effective counting time, which was renormalized to give 10^8 monitor counts (MON).

By dividing this expression for the data by a similar expression for the standard sample, ABS calculates the absolute cross-section for the data from:

$$d\sigma(Q)/\Delta\Omega = [I(Q) \text{ MONs } d_s T_s] / [I_s(0) \text{ MON } d T] [d\sigma_s(0)/\Delta\Omega]$$

where:

$I_s(0)$ = measured intensity of the standard sample at $Q=0$,

d_s = thickness of the standard sample and

T_s = measured transmission of the standard sample (which is wavelength dependent).

Note that if $I(Q)$ and $I_s(Q)$ are from radially averaged work files then $\text{MONs}=\text{MON}$.

Another, often simpler method for rescaling data to an absolute intensity consists in a direct measurement of the beam flux at the sample using the area detector. This measurement is similar to the empty beam measurement when measuring transmissions (move attenuators in and the beam stop out). The quantity $K = \Phi A \Delta\Omega \epsilon t$ is the scaling factor, automatically calculated as follows: ΦA is the total (empty beam transmission) detector counts per unit time/attenuation factor at the used wavelength, t is the counting time $\times 10^8/\text{MCR}$, and $\Delta\Omega$ is equal to $(0.5 \text{ cm/sample-to-detector distance in cm})^2$.

In some cases, it is not necessary to convert your data to absolute scale.

Masking the dataset

The last step before averaging the data to reduce it to I vs Q form is to mask the dataset. This operation has the effect of marking, or masking, specific pixels in the 2D data field that are to be ignored in the subsequent averaging process.

Averaging the dataset

At this point the corrected data can be reduced to I vs Q or saved in another format. Typically, the averaging operation is used to perform either a radial, angular, sector or rectangular average (ignoring all masked pixels) of the 2D data field to reduce it to I vs Q. The averaged data are stored in individually named ASCII (text) files. Data that have been converted to an absolute scale are, after averaging, stored in a file with the extension .ABS; otherwise, the results are stored in a file with the extension .AVE.

The final averaging step can also be set to save the reduced data in a 2D ASCII format. The 2D ASCII format can be re-read into the SANS Reduction package for further processing. See [2-D Work File Arithmetic](#).

SANS System Requirements

- Macintosh or PC
- IGOR Pro installed <http://www.WaveMetrics.com> (in 8/03, v. 4.0x is the current version). As of 10/2001, SANS Reduction macros require IGOR Pro v. 4.0x. As always, the macros will work with free Demo versions of IGOR.

NOTE: You DO NOT need to purchase IGOR Pro to reduce your data. You can use either the (free) Demo version of IGOR Pro, or the full version. IGOR 4.0x or higher is required. Some features are, however, unavailable in the Demo version. (The use of certain trade names or commercial products does not imply any endorsement of a particular product, nor does it imply that the named product is necessarily the best product for the stated purpose.)

- SANS Reduction Macros and the Tutorial data are available on our website: http://www.ncnr.nist.gov/programs/sans/manuals/data_red.html
Follow the instructions on the webpage for downloading and installing the SANS Reduction Macros.
- The output ASCII (I(q) vs. q) files are also compatible with a collection of models that can be fitted to your SANS data. These models are available at: http://www.ncnr.nist.gov/programs/sans/manuals/data_anal.html , and use IGOR Pro's curve fitting features.

What's New in SANS

Changes from Version 4 (10/2001) to Version 4.2 (08/2003):

Display enhancements

- SANS Menu items will open or make visible the most commonly used panels so that they can quickly be located on screen.

Export formats

- The currently displayed SANS Data, including fully or partially corrected data can be saved as 2D ASCII. This data can be directly read in and operated on using [2-D Work File Arithmetic](#).

New operations

- 1-D data plots are now controlled by a Plot Manager making it easier to load and append data to graphs, and to remove old data sets from Igor's memory. See [Plot Averaged Data](#).

- Subtraction of 1D datasets can be performed, as well as subtraction of constant backgrounds or simple rescaling of data. See [Subtract 1D Data](#).
- [2-D Work File Arithmetic](#) operations are simplified, reading in and generating 2D ASCII format.
- A Marquee menu operation will graph a vertical or horizontal selection of the SANS Data display. See [Marquee Operations](#).
- A [SANS Preferences](#) panel has been added to set parameters for non-standard experiments.

Improved functions

- Absolute scaling based on an empty beam measurement has been changed to improve accuracy.
- Protocols are now portable, and can be exported as a text file to be imported into a new experiment.
- Sort operation now allows rescaling of a single data set. See [Sort and Combine Averaged Datasets](#).
- Detector sensitivity files can be created for the NG1 SANS which has two beam stops.
- Bin Width during 1D averaging can be adjusted from default values as a [SANS preferences](#) item.
- During the COR step, files are checked for Transmission=1. Options to temporarily override are presented. The check can be turned off/on as a preference item.
- Schematics now can be generated in either log or linear intensity scale.
- Data is rescaled to correct for attenuation when a reduction protocol is executed, even if no subtractions are performed.
- Help buttons are available on most panels that will jump to the relevant help section.

Instructions for the Impatient

- 1) Open the "SANS_Reduction..." experiment and pick the data path
- 2) [List the Data Files](#)
- 3) [Calculate Transmissions](#)
- 3) [Build a Data Reduction Protocol](#)
- 4) [Reduce a File](#)
- 5) [Sort and Combine Averaged Datasets](#)
- 6) Write journal article

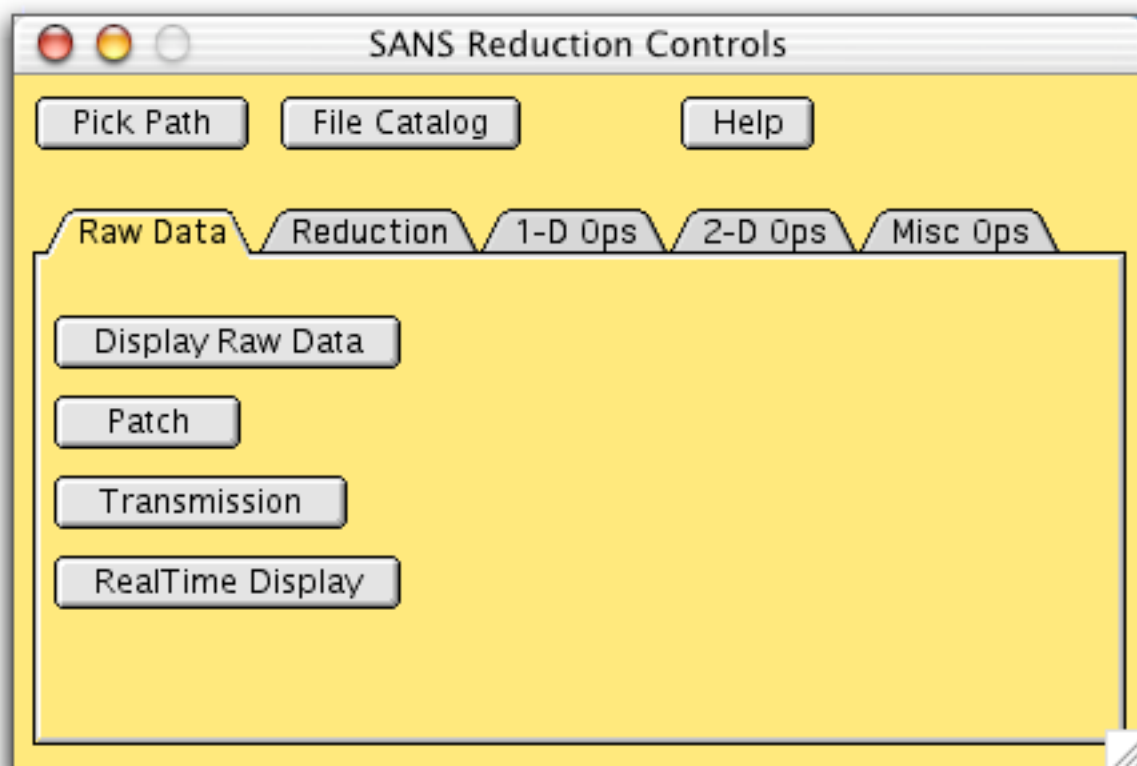
Tutorial Instructions

Main Controls

What: Upon opening a blank template experiment for SANS data reduction, this main control panel is the starting point for viewing your data, performing the data reduction, plotting the averaged data, and performing some simple analysis. It organizes the essential controls for SANS data reduction in one location.

How: The SANS Reduction macros are loaded and compiled automatically upon opening the "SANS_Reduction..." experiment. After successfully compiling, the Main Panel of SANS Reduction Controls is automatically created. If you've lost this panel on the screen, selecting

SANS->Initialize from the main menu bar will bring this window to the front. Clutter can be minimized by closing auxiliary panels when not in use. Panels are automatically re-created on demand.



The buttons are:
(always visible)

Pick Path: presents a dialog to select the folder that contains your data. This only needs to be set once, at the beginning of a data reduction session.

File Catalog: after the data path has been set, this will generate a table of information about each file in the data folder. The table is very useful to identify each file and for building reduction protocols.

Help: will display this help file.

There is also a SANS Menu that is always visible on the main menu bar. Menu selections will generate the input panels as if the corresponding button had been pressed on the Main Panel, or simply bring the window to the front if it has been misplaced. The Initialize step is run automatically as the experiment is launched, but can be re-run at any time to ensure that the SANS Preference values are reset to their default values. For a detailed description of the buttons contained on all of the tabs, see:

[Raw Data Tab](#)

[Reduction Tab](#)

[1-D Ops Tab](#)

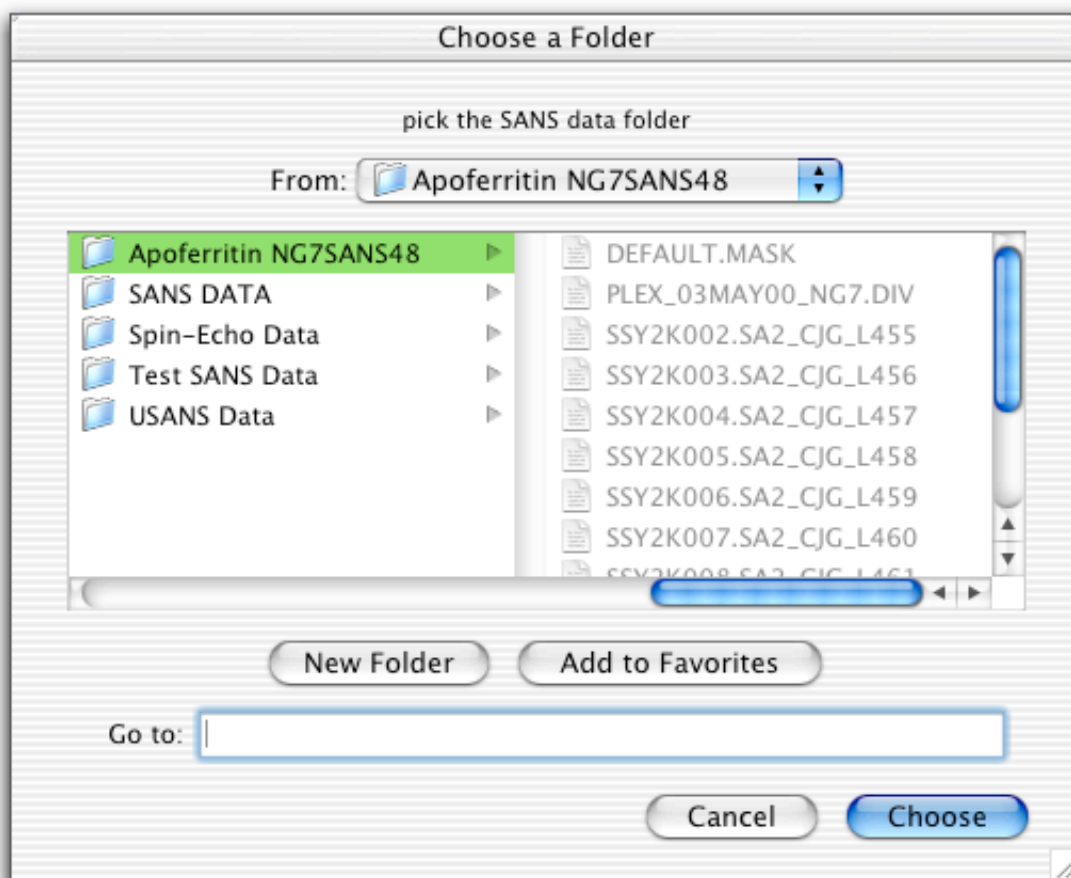
[2-D Ops Tab](#)

[Misc Ops Tab](#)

List the Data Files

What: Set a path to your data folder. Then create a "Catalog" table with information about your data files, available for use in building data reduction protocols.

How: All of the raw data files, detector sensitivity files, mask files, etc. must be kept in a single folder for IGOR to access them. From the main panel, click "Pick Path" to set the path to this folder. On a Mac, if your data is inside "Tutorial Data", the dialog should look like this. On Windows, the dialog will look slightly different.



Once the path is set, click "File Catalog" to create a catalog table listing of all of the files in the selected folder. Raw SANS data files will show descriptive header information like the label, counting times, and thickness and transmission. The columns can be resized to see the whole label, etc., or delete columns of information you don't want to see. This table is also used interactively for building data reduction protocols, and is detailed later. Clicking "File Catalog" again will rebuild the list of files, and should be done if files were added to the folder or to confirm that header information was updated correctly. The table will list all of the files in the data folder, displaying information about raw SANS data files only. Files that are not recognized as raw SANS data are appended to the bottom of the "FileNames" column. Note that in the "FileNames" column, there are two important files listed that are not raw SANS data - these are the mask and detector sensitivity files.

Data File Catalog						
ROCO		SSY2K002.SA2_CJG_L455				
Filenames	Labels	DateAndTime	SDD	Lambda	CntTime	TotCnts
SSY2K002.SA2	beam center 6m	7-JUN-2000	6	6	60	142196
SSY2K003.SA2	T. APOFERRITIN	7-JUN-2000	6	6	60	113014
SSY2K004.SA2	S. APOFERRITIN	7-JUN-2000	6	6	900	899006
SSY2K005.SA2	blocked beam 6r	7-JUN-2000	6	6	300	595
SSY2K006.SA2	buffer Sample 6	7-JUN-2000	6	6	300	26940
SSY2K007.SA2	T.empty 6m and	7-JUN-2000	6	6	60	113190
SSY2K008.SA2	T.beamcenter 1.	7-JUN-2000	1.6	6	60	9330
SSY2K009.SA2	s.apoferritin 1.	7-JUN-2000	1.6	6	900	4.20182e+
SSY2K010.SA2	blocked beam 1.	7-JUN-2000	1.6	6	900	4352
SSY2K011.SA2	buffer 1.6m and	7-JUN-2000	1.6	6	900	2.30794e+
DEFAULT.MASK						
PLEX_03MAY00						

The Display Window

What: Display a raw 2-D SANS data file and get some simple information about the data.

How: 2-D SANS data is displayed by clicking "Display Raw Data" under the Raw Data Tab on the Main Panel. A standard dialog is presented to select the raw data file. The data is displayed versus detector pixel (left and bottom axes) and versus Qx and Qy (top and right axes), along with a color scale. Important information about the data is displayed at the top of the graph, including the filename, the (X, Y) position of the cursor, and the count value. If the display type is "RAW" then this is the actual neutron counts for that pixel. If the displayed data is one of the correction steps, it may not be an integer neutron count value. The horizontal, vertical, and total q-values (in Angstroms⁻¹) are also displayed. Further information about the file can be displayed by clicking the "Status" button, and the information is printed to the command window at the bottom of the screen. The color mapping of the detector counts can be toggled between logarithmic and linear scale by clicking the "isLin" button. The current label on the button, either "isLog" or "isLin" gives the current scaling. The displayed data can be averaged (without doing any reduction steps) by clicking the "I vs. q" button. This will present a new panel with the [Average Options](#). For averages of sectors or slices of the 2D dataset, the region to be averaged is marked on the dataset in response to the angles and widths chosen in the panel. The defaults are for a standard circular average of the full dataset.

If the data displayed is "RAW" data, and a path to the data has been chosen, left and right arrow buttons will also be present on the graph. This will display the next (or previous) run number in the data folder, if available, without having to proceed from the main panel through an open file dialog to select the file. The Color Map sliders can be adjusted as desired to alter the color display of the data.

The controls are:

Status: prints selected information about the displayed file to the command window at the bottom of the screen.

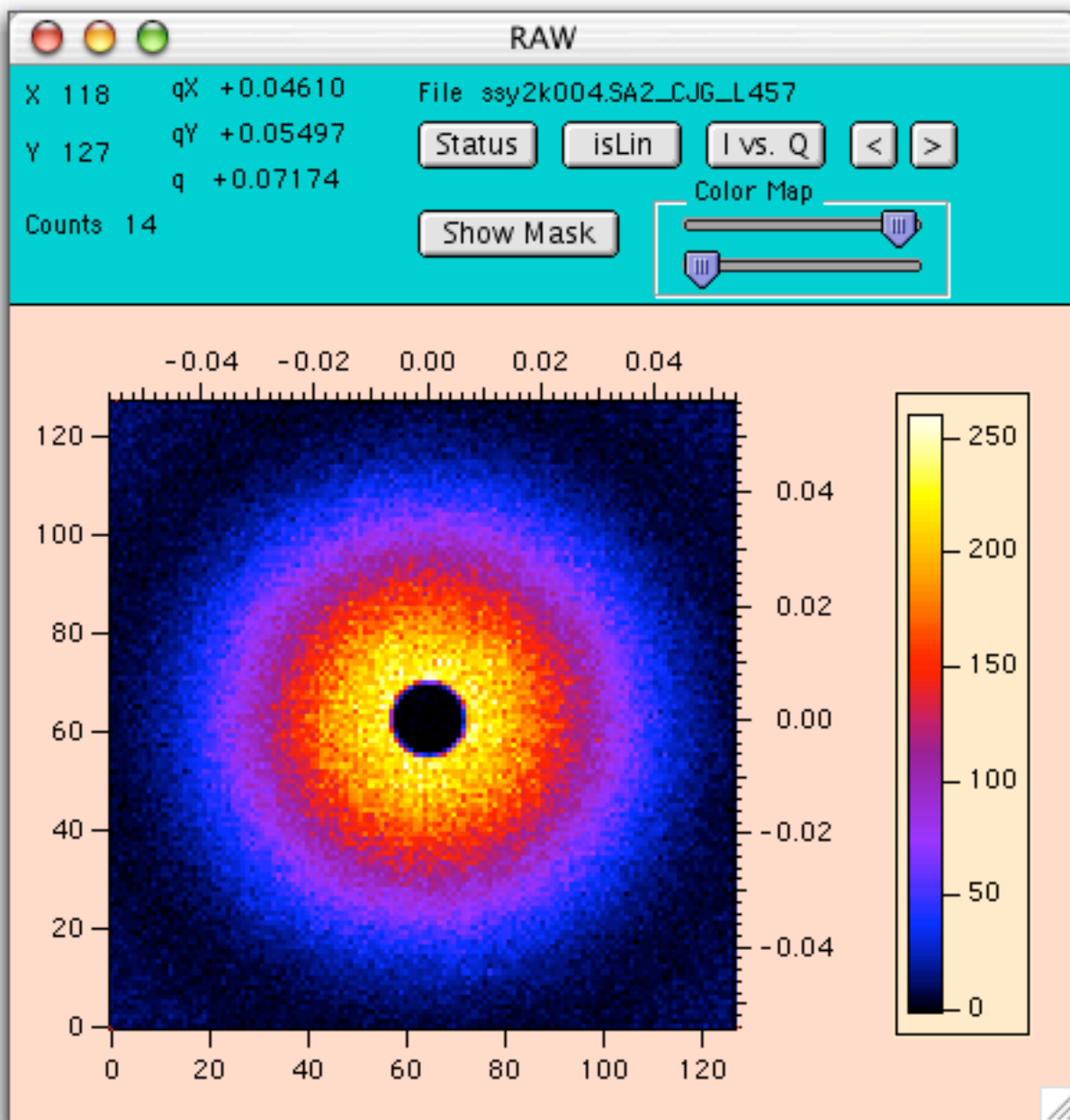
isLin: toggles the color map scaling of the detector counts from linear to logarithmic. When the data is log-scaled, the button will read "isLog".

I vs. Q: displays a new panel with averaging options to produce a 1-D averaged dataset of the 2-D data, or save the data in a 2D format. No reduction steps are performed.

Left/Right Arrows: are only visible if the displayed data is "RAW" data. If the data path has been set, these buttons will increment the display to the next (or previous) run number, bypassing the open file dialog.

Show Mask: toggles the currently loaded mask file (if present) on/off the dataset in a bright green color, indicating which data points are to be excluded from the 1-D average.

Color Map Sliders: adjust the upper and lower threshold limits for the color scale to highlight features in the 2-D detector image.



Average Options

What: This feature allows you to perform different types of averages on your data, and allows you to see what regions of the detector will contribute to the average. Open the Average Panel, and try out some different types of averages. The regions to be averaged are clearly shown on the data, and can be easily adjusted. The numerical values of pixels, angles, etc. can be used later in reduction protocols.

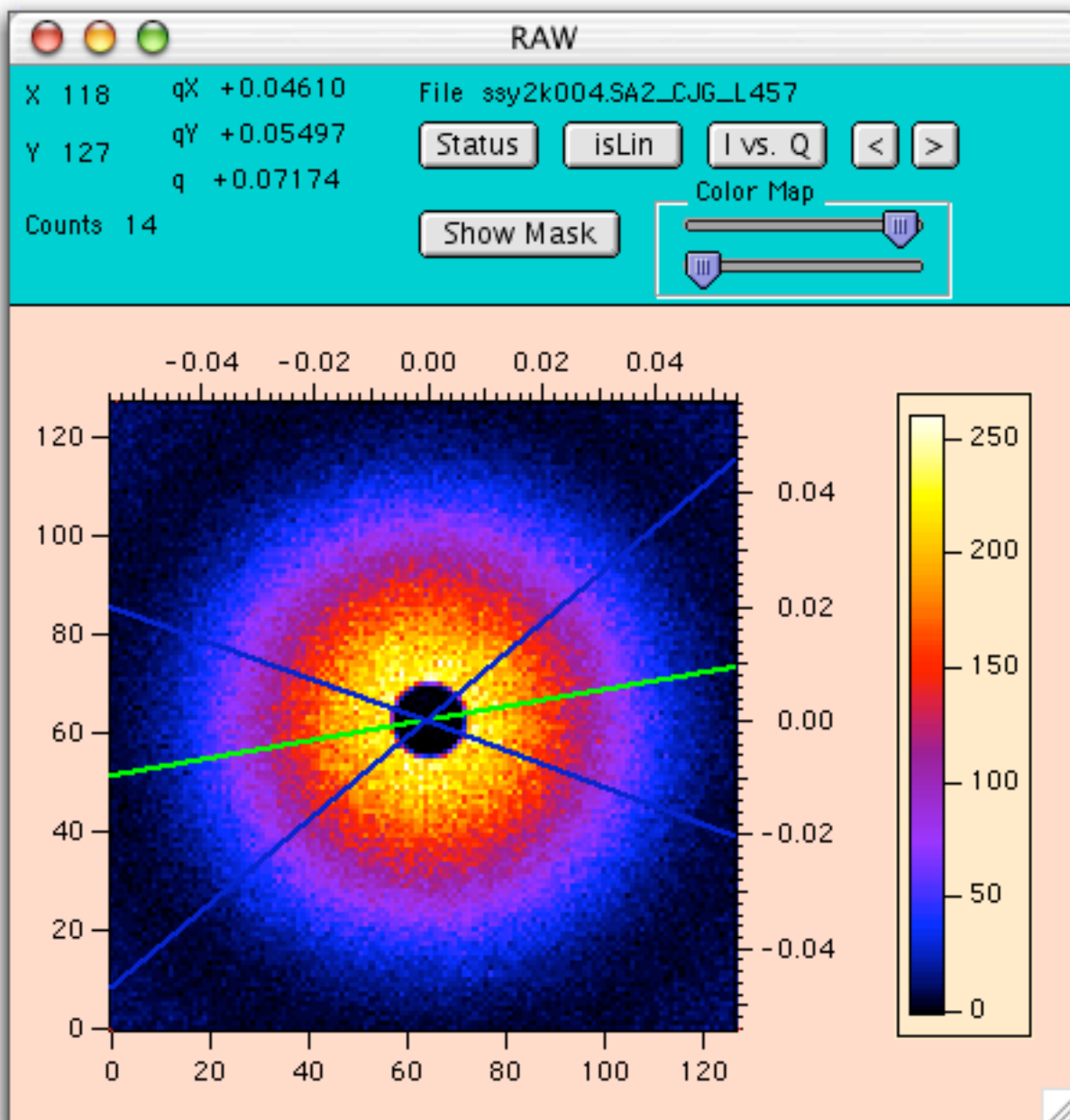
How: Open the Average Panel either using the "I vs Q" button on the Display window, or the "Average" button on the Misc Ops tab of the main panel. You will then be able to average whatever data is currently in the display.

- "Circular" is the default average type. It will perform and average in constant q-rings around the (x,y) pixel location of the beam center. The default pixel width is fixed at one, and there are no other options to set when doing a circular average.
- "Rectangular" will average in constant q-arcs, but limited to a rectangular swath of a specified width of pixels. This rectangular swath can be oriented at any angle, and include either side or both sides of the detector.
- "Sector" is very similar to Rectangular, except that the width of the sector is specified in degrees (+/- delta phi) each direction from the central angle (phi).
- "Annular" will perform an average centered at a single q-value (q-center), and averaged over a width of a specified number of pixels. The data is returned as a function of angle (phi) in degrees. If a normal x-y coordinate system is drawn through the beamcenter, zero angle corresponds to the positive x-axis and proceeds counter-clockwise. Therefore 270 degrees corresponds to the negative y-axis.
- "2D ASCII" saves the currently displayed data in 2D form in terms of intensity versus pixel coordinates. This data can be re-read using the [2-D Work File Arithmetic](#) Panel to perform further processing steps.
- "QxQy ASCII" saves the currently displayed data in 2D form in a three column format, converting each detector pixel into Qx and Qy and its corresponding intensity. This data format cannot be re-read into the SANS macro set.

For this selection of sector average, and the angles phi and delta phi:

The screenshot shows a dialog box titled "Average_Panel" with a pink background. At the top, "AverageType" is set to "Sector" with a dropdown arrow and a help button "?". Below this, there are four panels for different average types: "Sector/Rectangular", "Annular", "Rectangular", and "Sector". The "Sector/Rectangular" panel is active, showing "Sides ?" set to "both" and "Phi" set to "10". The "Annular" panel shows "Q-center" set to "0" and "Q Delta" set to "1 (pixels)". The "Rectangular" panel shows "Width" set to "1 (pixels)". The "Sector" panel shows "Delta Phi" set to "30". At the bottom, there is a checkbox "Save file to disk?" which is unchecked, and four buttons: "Do Average", "Clear", "Done", and a small icon button in the bottom right corner.

The corresponding Display shows what data will be included. The green line is the center of the average (ϕ) and the blue lines are maximum extent of the sector ($\Delta\phi$), ± 30 deg = 60 degrees total angle.



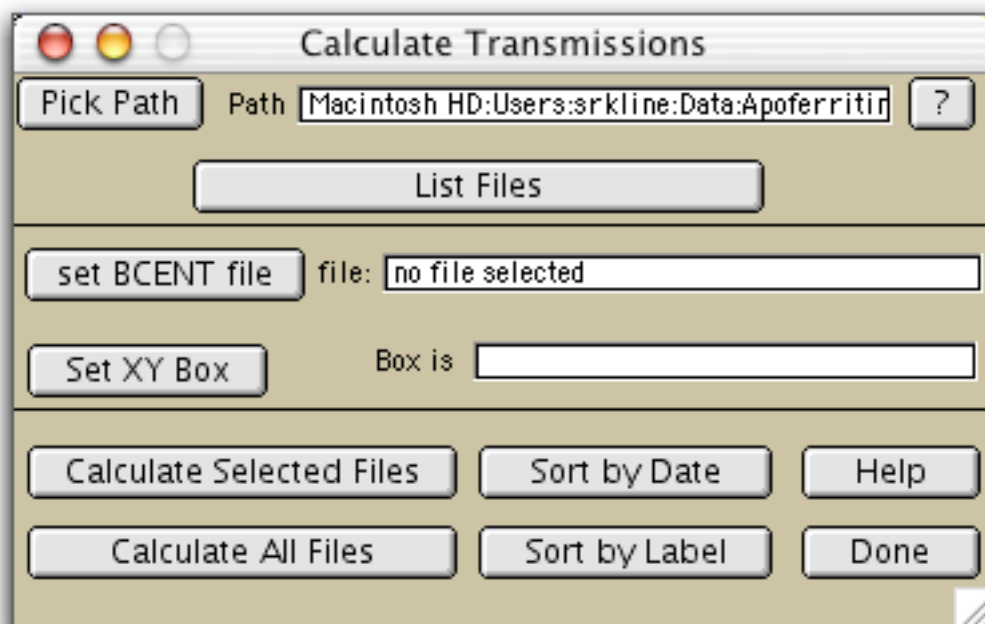
Averaged data that has been saved from this panel (only if "Save File to disk?" is checked) will have "unknown" files listed as its protocol, since there's no way of knowing what steps have been performed on the 2-D data. If you know what you've done to the data, you're ok - it's just there as a warning.

For Circular, Sector, and Rectangular averages, the data is binned in a width of one pixel as default. For Annular averages, the circle of 2π is broken into 72 bins as default. These values can be changed using the [SANS Preferences](#) panel.

Calculate Transmissions

What: Transmission of samples and sample containers must be calculated and entered into the headers of the raw data files for proper subtraction of non-sample scattering during data reduction. Here we will create the "associations" between the transmission measurements and the scattering files to which they correspond. Transmissions will then be calculated and automatically patched to the file headers.

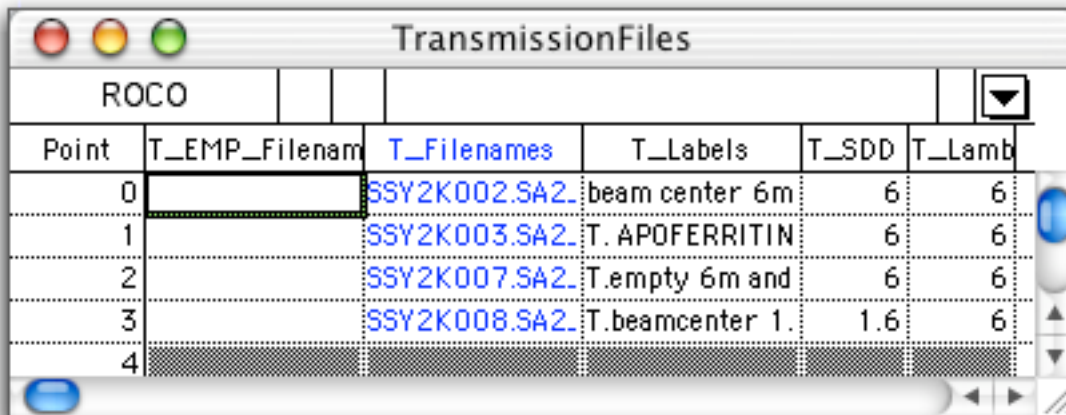
How: 1) Open the Transmission panel by clicking "Transmission" on the Raw Data tab of the main panel. The following new panel will appear:



2) Click on "List Files" to build two tables - one with scattering files:

Point	S_TRANS_Filename	S_Filenames	S_Labels	S_SDD	S_Lamb	S_Trans
0		SSY2K004.SA2	S. APOFERRITIN	6	6	1
1		SSY2K005.SA2	blocked beam 6r	6	6	1
2		SSY2K006.SA2	buffer Sample 6	6	6	1
3		SSY2K009.SA2	s.apoferritin 1.	1.6	6	1
4		SSY2K010.SA2	blocked beam 1.	1.6	6	1
5		SSY2K011.SA2	buffer 1.6m and	1.6	6	1

and another with transmission files. The transmission files are automatically separated from the scattering files based on the beamstop location (off-center) in the header of the raw data file.

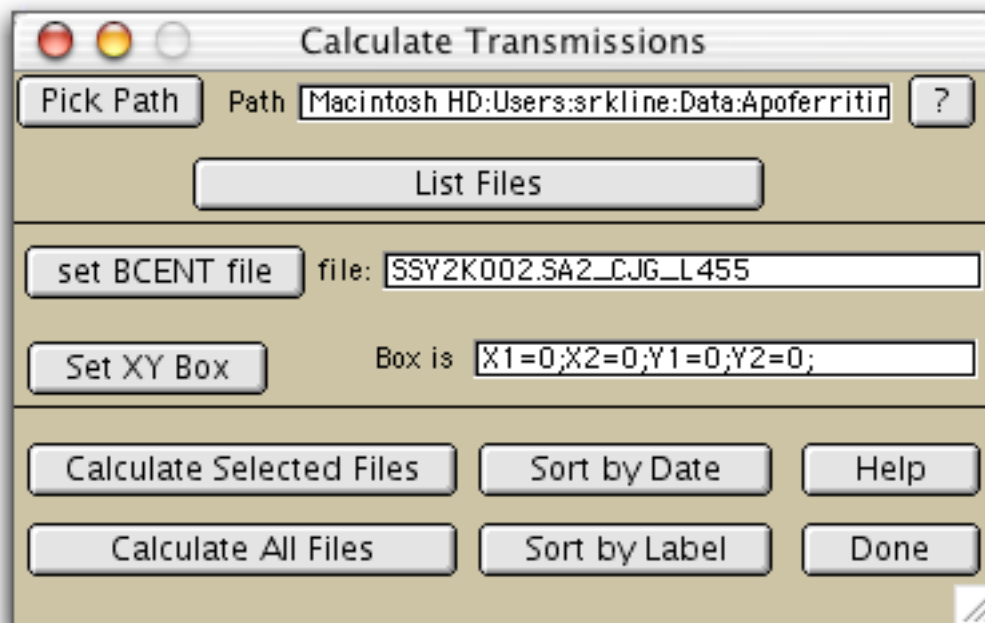


TransmissionFiles

ROCO

Point	T_EMP_Filenam	T_Filenames	T_Labels	T_SDD	T_Lamb
0		SSY2K002.SA2	beam center 6m	6	6
1		SSY2K003.SA2	T. APOFERRITIN	6	6
2		SSY2K007.SA2	T.empty 6m and	6	6
3		SSY2K008.SA2	T.beamcenter 1.	1.6	6
4					

3) Find the empty beam transmission measurement in the TransmissionFiles table. It is in the blue "T_Filenames" column. For the tutorial, it is file SSY2K002.SA2..... Click on this file to select it (just that cell in the table). In the Transmission Panel, click "Set BCENT File" to set this file as the empty beam. The filename appears, as well as the box coordinates:



Calculate Transmissions

Pick Path Path Macintosh HD:Users:srkline:Data:Apoferritin ?

List Files

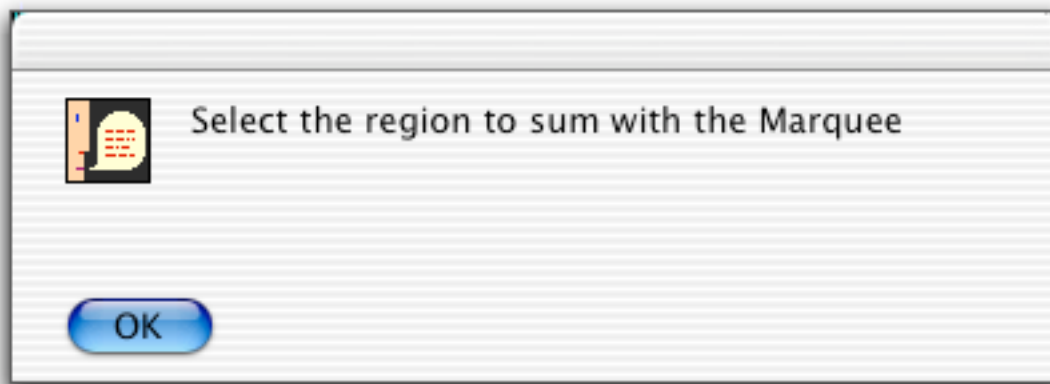
set BCENT file file: SSY2K002.SA2_CJG_L455

Set XY Box Box is X1=0;X2=0;Y1=0;Y2=0;

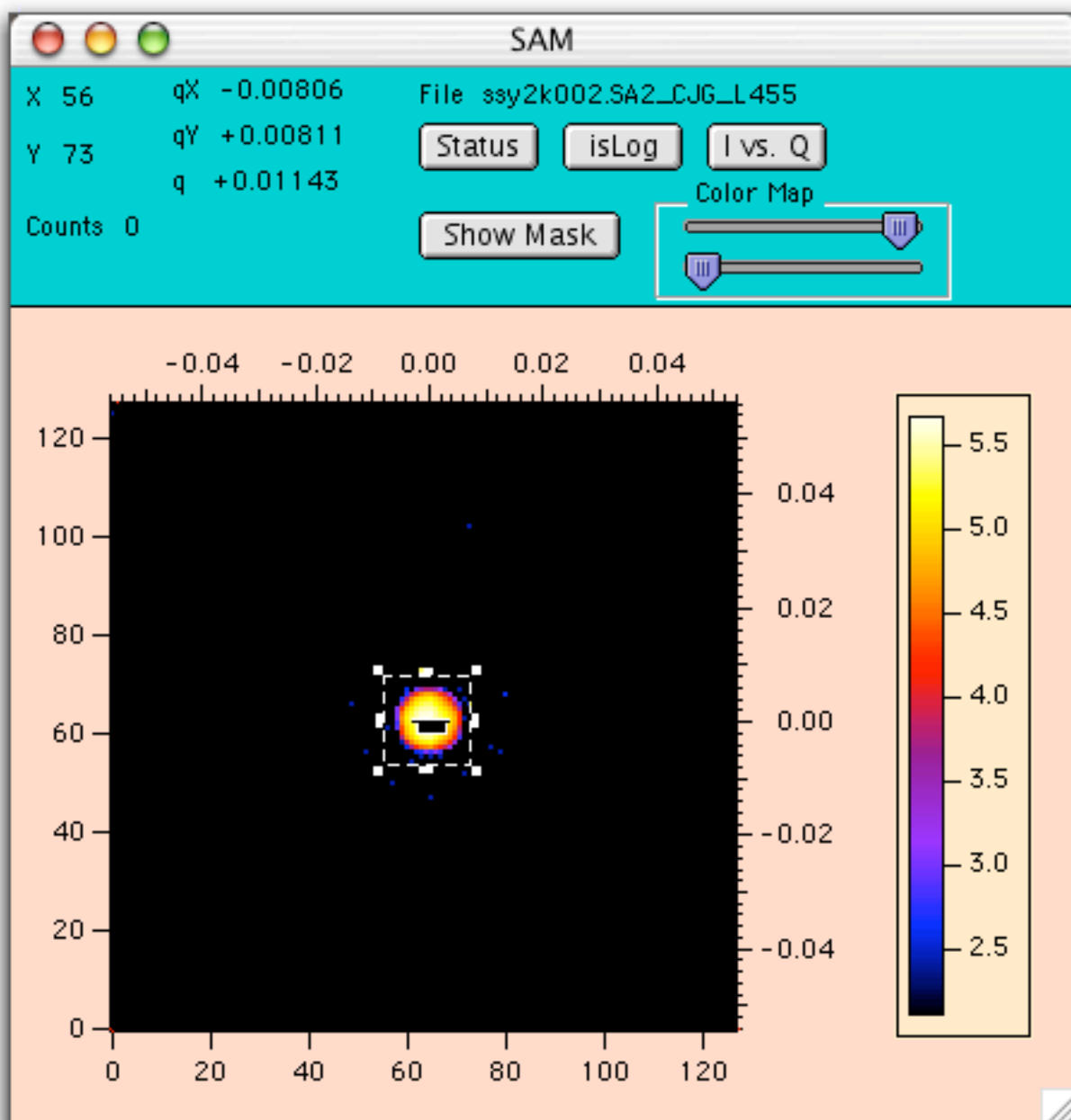
Calculate Selected Files Sort by Date Help

Calculate All Files Sort by Label Done

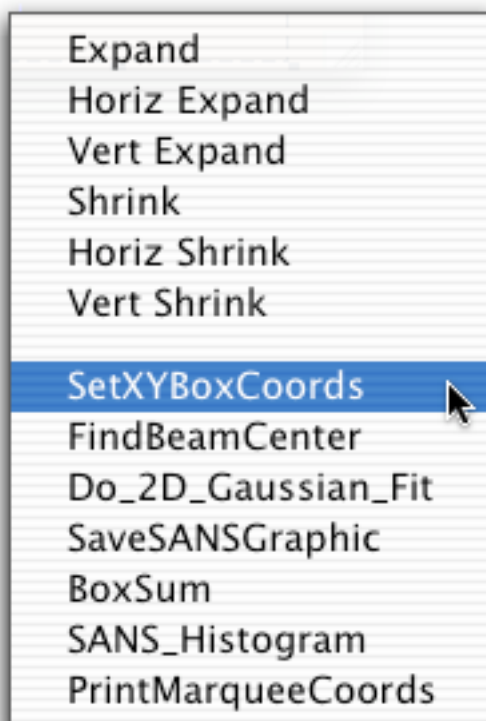
The "intensity" of the empty beam is found by summing the number of counts on the detector over a specific rectangular region of the detector. Currently the box coordinates are zeros, so we need to pick the rectangle. Do this by clicking "Set XY Box". The raw data file (SSY2K002) will be displayed, and you will be presented with the following dialog:



In the data display, click and drag a marquee that encompasses the primary beam. You may find it easier to see the full extent of the beam if you switch the display to log scale. Move the cursor inside the marquee, to get an "upside-down hat" cursor.

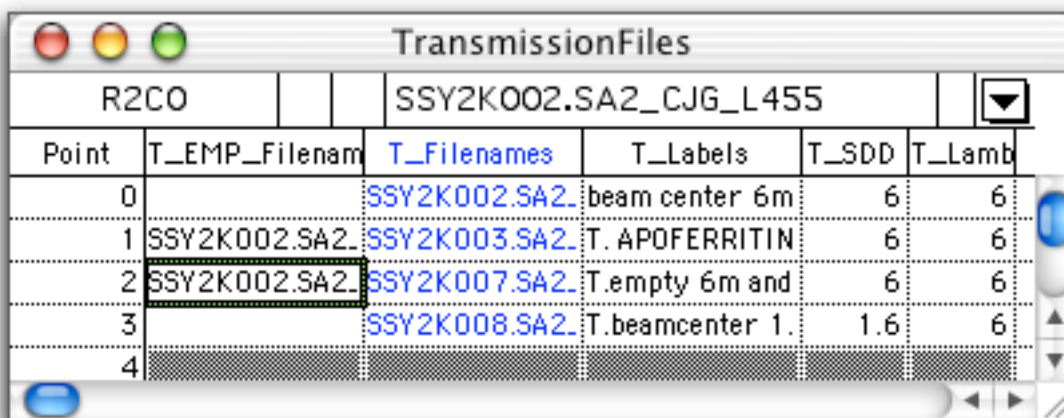


Click to get a menu, and near the middle, select "Set XY Box Coords".



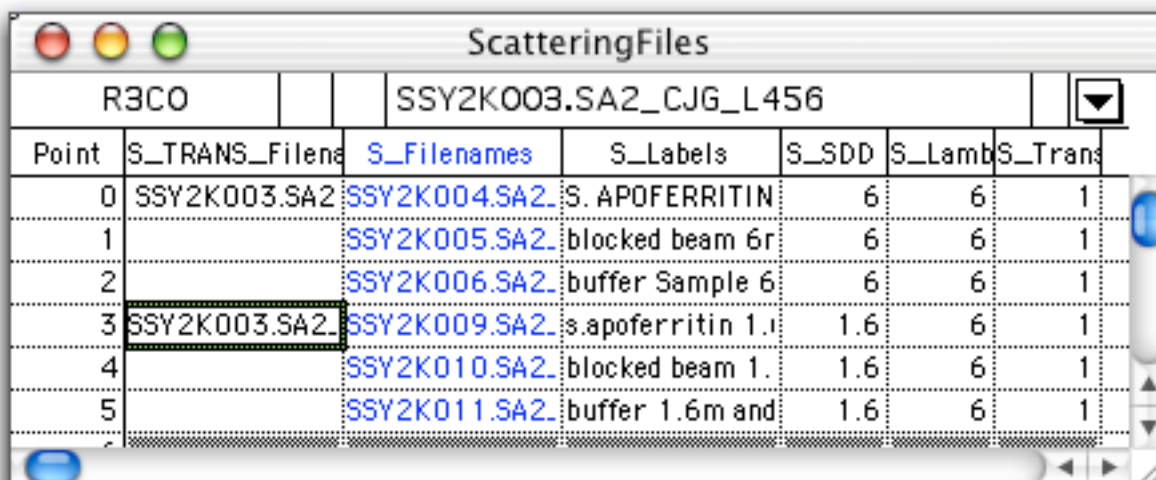
The pixel values for the box will be updated to the Transmission panel, and are written to the empty beam file header for future calculations. You won't need to do this again. Note that the marquee selection can also be used to measure the beam center, or centroid of any selected region. See [Marquee Operations](#) for more details.

4) Now make the associations between the empty beam file and each of the transmission measurements. Each transmission measurement for a sample must be normalized relative to the empty beam transmission (and should therefore be less than unity). Make the EMPTy beam association by selecting the empty beam file (in the blue column), copying it, and pasting the filename into the "T_EMP_Filename" column. You obviously don't need to associate the empty with itself, or with the beamcenter measurement that was taken at a different sample-to-detector distance (T_SDD). Transmission was only measured of two samples: the apoferritin (a protein in an aqueous buffer, held in a quartz cell), and the buffer alone in the same cell. Note that the sample label says "T. empty...", but it's really the buffer. You should try to do better with your sample labels. The TransmissionFiles Panel should look like this:



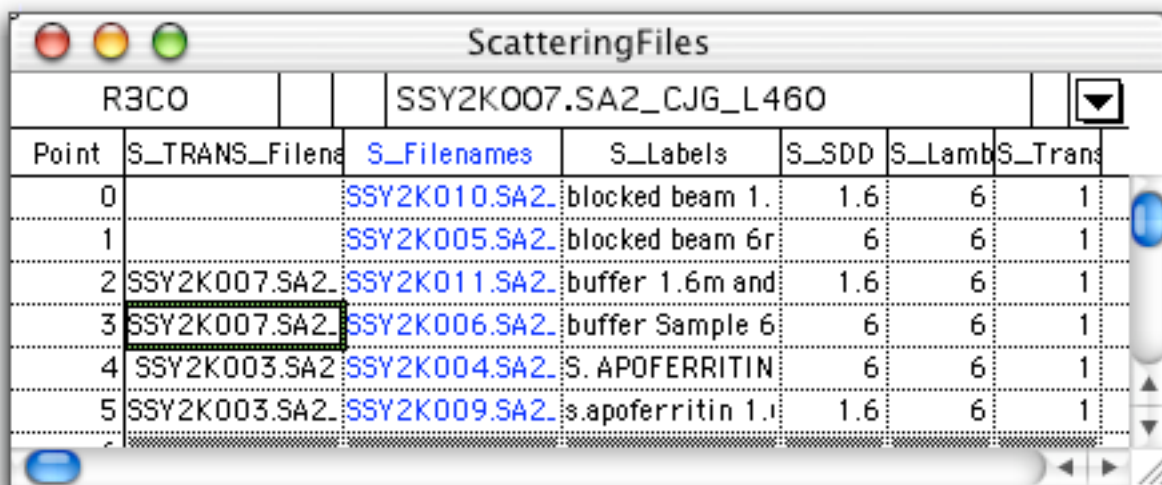
Point	T_EMP_Filename	T_Filenames	T_Labels	T_SDD	T_Lambda
0		SSY2K002.SA2	beam center 6m	6	6
1	SSY2K002.SA2	SSY2K003.SA2	T. APOFERRITIN	6	6
2	SSY2K002.SA2	SSY2K007.SA2	T.empty 6m and	6	6
3		SSY2K008.SA2	T.beamcenter 1.	1.6	6
4					

5) Now make the association between the transmission measurement of the apoferritin (SSY2K003) and the scattering file(s) for the same sample. In this case, the apoferritin scattering was measured twice - using two different instrument configurations. The sample is the same, and so is the transmission, so copy the filename of the apoferritin transmission (SSY2K003...) from the blue "T_Filenames" column, and paste it into the (2) proper locations in the "S_TRANS_Filenames" column in the ScatteringFiles table, like this:



Point	S_TRANS_Filename	S_Filenames	S_Labels	S_SDD	S_Lambda	S_Trans
0	SSY2K003.SA2	SSY2K004.SA2	S. APOFERRITIN	6	6	1
1		SSY2K005.SA2	blocked beam 6m	6	6	1
2		SSY2K006.SA2	buffer Sample 6	6	6	1
3	SSY2K003.SA2	SSY2K009.SA2	s.apoferritin 1.	1.6	6	1
4		SSY2K010.SA2	blocked beam 1.	1.6	6	1
5		SSY2K011.SA2	buffer 1.6m and	1.6	6	1

If you were consistent in your sample labels, it is often more convenient to group the same samples together, rather than a chronological listing of the scattering files. Click the "Sort by Label" button in the Transmission Panel to get the following listing - note that the previous associations are carried along, and now the scattering measurements are conveniently grouped together. Do the same copy-paste (one at a time only) of the buffer transmission file (SSY2K007...) into the appropriate locations in the ScatteringFiles table. Note that there are no transmission files assigned for the blocked beam. We know that's zero, and the data reduction steps take care of that automatically. It doesn't matter if the file thinks that the transmission is one (like it does currently). The ScatteringFiles table should look like this:

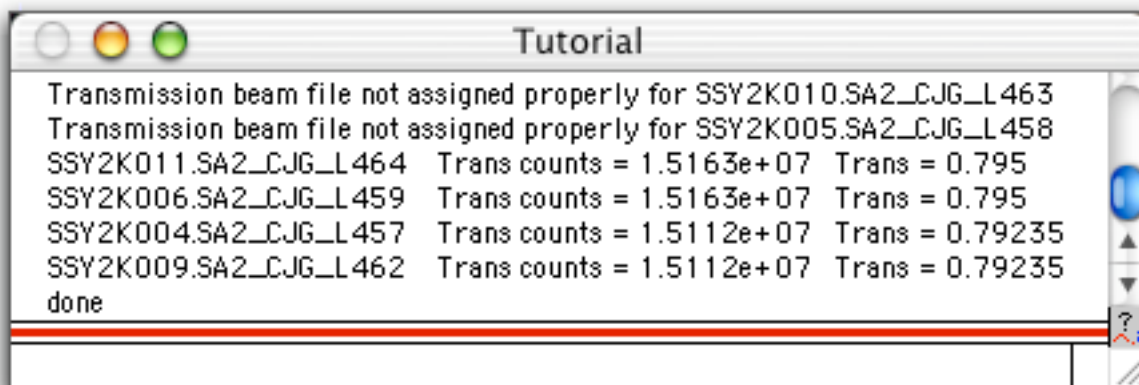


ScatteringFiles

R3CO SSY2K007.SA2_CJG_L460

Point	S_TRANS_Filename	S_Filenames	S_Labels	S_SDD	S_Lambda	S_Trans
0		SSY2K010.SA2	blocked beam 1.	1.6	6	1
1		SSY2K005.SA2	blocked beam 6r	6	6	1
2	SSY2K007.SA2	SSY2K011.SA2	buffer 1.6m and	1.6	6	1
3	SSY2K007.SA2	SSY2K006.SA2	buffer Sample 6	6	6	1
4	SSY2K003.SA2	SSY2K004.SA2	S. APOFERRITIN	6	6	1
5	SSY2K003.SA2	SSY2K009.SA2	s.apoferritin 1.	1.6	6	1

6) All of the proper associations have been made, so it's time to calculate the transmissions. "Calculate All Files" is the obvious choice from the Transmission Panel. The results of the calculation are displayed in the command window (usually at the bottom of the screen, cmd-J or ctrl-J will bring it to the front). The transmission files were not assigned properly for SSY2K010... and SSY2K005... which is not a problem, since these are our blocked beam files and we don't calculate the transmission of these files anyways. The other four transmissions are calculated correctly, and these transmission values are automatically patched to the raw file headers, and updated to the ScatteringFiles table. The File Catalog table, however, is not updated (unless you force it to update by clicking File Catalog on the main panel again).



Tutorial

```

Transmission beam file not assigned properly for SSY2K010.SA2_CJG_L463
Transmission beam file not assigned properly for SSY2K005.SA2_CJG_L458
SSY2K011.SA2_CJG_L464  Trans counts = 1.5163e+07  Trans = 0.795
SSY2K006.SA2_CJG_L459  Trans counts = 1.5163e+07  Trans = 0.795
SSY2K004.SA2_CJG_L457  Trans counts = 1.5112e+07  Trans = 0.79235
SSY2K009.SA2_CJG_L462  Trans counts = 1.5112e+07  Trans = 0.79235
done

```

7) Transmission calculations are done. Clicking done will remove the panel and both tables. All of the tables and associations are regenerated by starting again from the "Transmission" button on the main panel. The previous associations are retained, and newly collected data files will have no associations. If the empty beam file had been previously set, it does not need to be set again, no matter what the panel indicates. Re-"setting" the EMPTy file as in step 3 will show that the box coordinates are not zeros, but are the coordinates that you previously selected with the marquee. In addition, if you only want to calculate the "new" files, select them in the blue "S_Filenames" column, and "Calculate Selected Files". It won't hurt to calculate all of the files, but it is a waste of time.

Patch File Headers

What: Some of the information in the file header may have been incorrectly set at the time of data collection, and must be updated before data can be correctly reduced. Here we can change header values in the raw data files. Typically, no information needs to be changed here, since transmission values were automatically "patched" by the Calculate Transmission step.

How: From the Raw Data tab on the main panel, click "Patch". This will display a new panel that can be used to verify and change certain fields in the raw data headers. If the data path is not set, do it now using the "Pick Path" button. Click (and release) the popup menu of files to refresh the list. Since the Match String is "*", all data files will be shown. The "*" has the usual wild-card meaning. Only a single wildcard can be used to trim the list of files displayed in the popup. The header information in the displayed file in the popup is shown below it in the text fields. If, for example, you want to change the sample label, you simply enter the new text into the box, check the "change" box next to it, and click "change header". If the "change" box is not checked, that field cannot be changed in the file header. This feature prevents accidentally changing values you don't intend to change. To patch the same information to a series of data files (like the beam center X and Y) enter the new values and check the "change" boxes. You can use the match string to trim the file popup to include the files that you want to change (you may have to change the files in a few batches to change just the ones you want). Then click "change all headers in list". You will be warned that it will change more than just the top file, and say "yes" to change all the files in the list. Transmissions were calculated previously using the Transmission panel, and should all be correct here.

Patch Raw SANS Data Files

Pick Path Path ?

File(s) to Patch Show Header

Match String Change Header

Change All Headers in List

Change?

☐ label

☐ Transmission

☐ Thickness (cm)

☐ Beamcenter X

☐ Beamcenter Y

☐ Attenuator number

☐ Counting time (s)

☐ Monitor count

☐ Detector count

☐ Trans. det. count

☐ Wavelength (Å)

☐ Wavelength spread

☐ Temperature (C)

☐ Magnetic field (G)

☐ Source aperture (mm)

☐ Sample aperture (mm)

☐ Source to sample distance (m)

☐ Detector offset (cm)

☐ Beamstop diameter (mm)

☐ Sample to detector distance (m)

File Catalog Done Patching

Build a Data Reduction Protocol

What: Building and saving a protocol allows you to repeatedly reduce raw data files for a given configuration using the same exact sequence of corrections. Here, you can identify the files and steps necessary to correct your data for non-sample scattering, detector sensitivity, convert to absolute scaling, eliminate "bad" detector pixels, and produce output

in a variety of formats. Once a protocol is constructed for a specific instrument configuration, it can be saved and recalled for later use.

How: Click "Build Protocol" on the Data Reduction tab of the main panel. This will present a new panel with a list of reduction steps that can be used. Steps that are checked will be performed, steps that are not checked will be skipped (except that you will always supply a sample file, or be prompted for one). For this example, we will use nearly all of the data reduction steps, and first build a protocol to reduce data taken at a 6 meter sample to detector configuration and use absolute scaling from an empty beam measurement. Click "Show File Catalog" to bring the listing of files to the top, and arrange the windows so the list and the panel are visible.

1) Leave the sample field as "ask" so that the program will prompt us for the sample data file(s) when they are needed. We could specify a file to bypass the dialog, if desired.

Data Reduction Protocol

File Catalog Show File Catalog ?

☒ Sample set SAM file
file: ask

☒ Background set BGD file
file: ask

☒ Empty Cell set EMP file
file: ask

☒ Sensitivity set DIV file
file: ask

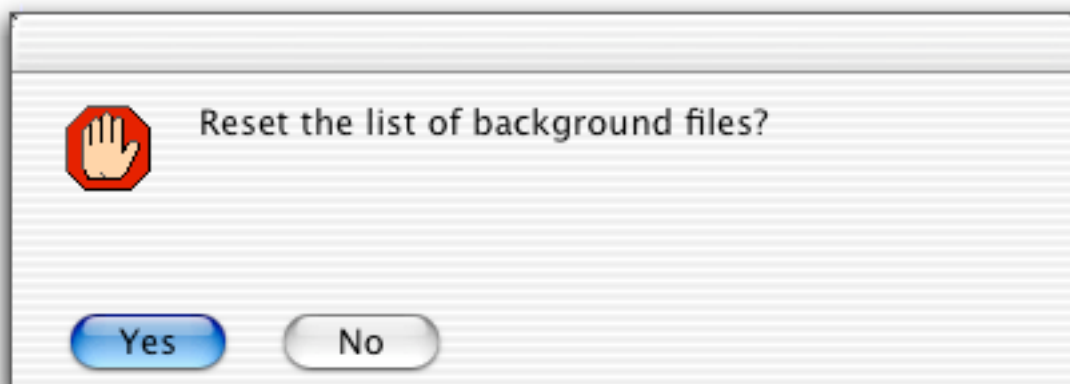
☒ Absolute set ABS params
parameters: ask

☒ Mask set MASK file
file: ask

☒ Average set AVERAGE params
parameters: AVTYPE=Circular;SAVE=Yes;NAME=A

Save Protocol Export Reduce A File
Recall Protocol Import
Delete Protocol Done

2) Fill in the background file by finding it in the listing (run SSY2K005), clicking to select the filename, and then clicking "Set BGD file" on the panel. The following dialog appears:

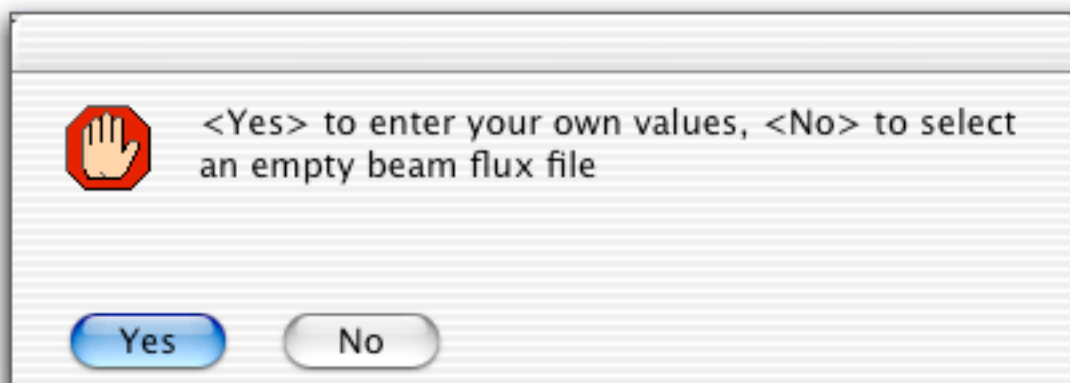


Say "Yes" to reset the list of files. This will set this single file (the selected text) as the background file. If several background files were collected and it is desired to add them together, reset the list for the first file, and then select "No" (don't reset) for additional files to add together. These additional files will be listed in the field as well and added together during the data reduction. The EMP (and SAM) file fields are set in an identical fashion.

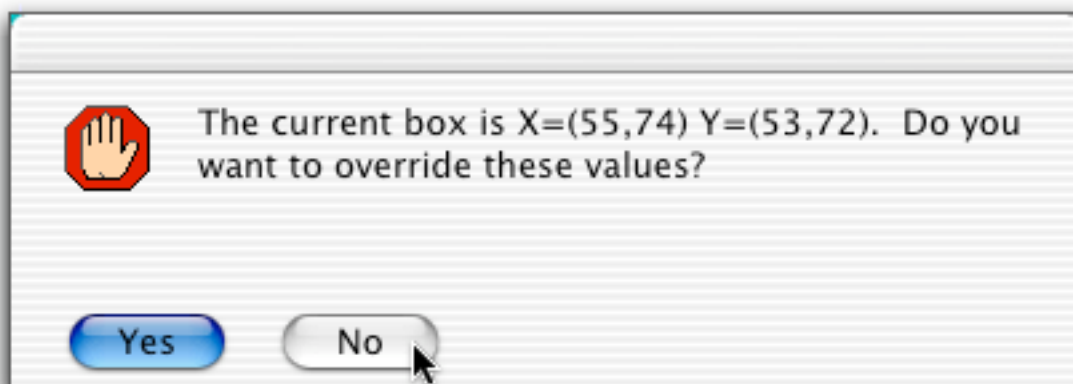
3) Fill in the EMPTy cell file (actually the buffer solution, in this example) in the same way that the BGD file was set. It is run SSY2K006.

4) Set the detector sensitivity (DIV) file. The file is PLEX_03MAY00_NG7.DIV (at the bottom of the Data File Catalog table). Note that it is not a raw SANS data file, and is not recognized as such by the listing. There can only be one detector sensitivity file assigned to a protocol.

5) Set the absolute scaling parameters. Click the "set ABS params" button, and the following dialog appears:

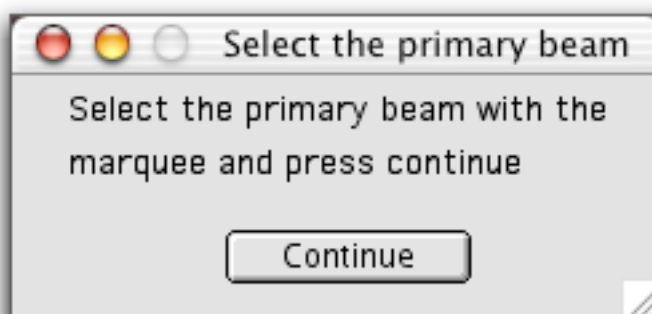


If you are using a measured secondary standard for calibration, "Yes" will allow you to enter your own values (i.e. the standard thickness, transmission, $I(q=0)$, and the tabulated cross-section of the standard sample). In this case, select "No" and you will be prompted for an empty beam measurement (at 6 meters) to use for absolute intensity calibration. When the dialog appears, select run SSY2K002..., which is the empty beam measurement. The file will be opened, and you will be prompted to keep or override XY coordinates. This is the box encompassing the direct beam that you set during the calculation of the transmission. This is exactly the same region you want to sum over for absolute scaling, so click "no" to accept these values.



You will (may) next be prompted with a dialog to open a file. It is asking for the detector sensitivity file (DIV), as stated in the title of the dialog. The DIV file is needed for the calculation of the absolute scaling factor, so select PLEX_03MAY00_NG7.DIV from the dialog, and open it. Now, with all information at hand, the scaling factor, kappa, is calculated and written both to the command window and to the text field in the Protocol Panel.

If you had not selected an XY box in the empty beam file, you would be presented with the following dialog (this will happen when you set up the protocol for the 1.6 meter configuration). Simply drag a box encompassing the primary beam, and click continue to dismiss the panel. Do not set the XY box using the marquee menu - it is not necessary for this step. Simply click Continue. The value of kappa and your box coordinates will be written to the command window.



6) Returning to the Protocol Panel, click on the "DEFAULT.MASK" filename in the listing, which is a simple mask to exclude the edges of the detector. Click "set MASK" to set the filename. The mask file was created either in IGOR Pro or in SANS Image. Note that this is NOT the same format as a "WORK.MSK" file from the VAX.

7) Default values for a circular average of the data (annulus width is always one pixel) should already be in the field. If not, or a different average is desired, click "set Average Params", and set the desired values in the dialog. Note that 2-D ASCII export formats or a save of the SANS graphic are regarded as "Average Types" since this is the protocol step where reduced data is written to disk. Of course, some of the fields do not apply for a given type of average, and their values are ignored.

The 'GetAvgInfo' dialog box contains the following settings:

Parameter	Value
Type of Average	Circular
Save files to disk?	Yes
Auto-Name files?	Auto
Plot the averaged Data?	Yes
Include detector halves?	both
Orientation Angle (-90,90) degrees	0
Azimuthal range (0,45) degrees	10
Width of Rectangular average	10
q-value of center of annulus	0.01
Pixel width of annulus	10

Buttons at the bottom: Quit Macro, Continue, Help

8) Once all fields are set to their correct files / parameters, click "Save Protocol" to save these settings for later recall, using a descriptive name for the protocol. "sdd_6meters" is a good choice for this protocol. Your Protocol Panel should look like this:

Data Reduction Protocol

File Catalog Show File Catalog ?

☒ Sample set SAM file
file: ask

☒ Background set BGD file
file: SSY2K005.SA2_CJG_L458,

☒ Empty Cell set EMP file
file: SSY2K006.SA2_CJG_L459,

☒ Sensitivity set DIV file
file: PLEX_03MAY00_NG7.DIV,

☒ Absolute set ABS params
parameters: TSTAND=1;DSTAND=1;IZERO=3262;

☒ Mask set MASK file
file: DEFAULT.MASK,

☒ Average set AVERAGE params
parameters: AVTYPE=Circular;SAVE=Yes;NAME=A

Save Protocol Export Reduce A File
Recall Protocol Import
Delete Protocol Done

9) Set up another protocol to reduce the data at the 1.6 meter configuration. This involves selecting a different background file, empty cell (buffer) file, and empty beam file for absolute scaling. The mask and detector sensitivity files do not need to be changed, nor do the averaging options. This time, we will use a (faster) method for "setting" the files for each step. The BKG file for 1.6 meters is SSY2K010. Simply highlight the filename field in the panel, and type the run number, 10 (leading zeros are not needed). You do not need to click the "set" button, simply enter the number. Run SSY2K011 is the buffer scattering, so enter 11 for the EMP file. Then set new ABS parameters in the same way as you did previously in step 5. Save this protocol as "sdd_1_6meters" or something else descriptive. Before saving the protocol, the run numbers are parsed into filenames, and the Protocol Panel should now have the following information. If a file could not be parsed, you would be informed of the offending number. Note also that multiple (and non-consecutive) runs can be added together

by simply typing a comma-delimited list of run numbers. Dashes can be used to represent inclusive ranges. See [Reduce Multiple Files](#) for an example.

Data Reduction Protocol

File Catalog Show File Catalog ?

☒ Sample set SAM file
file: ask

☒ Background set BGD file
file: SSY2K010.SA2_CJG_L463,

☒ Empty Cell set EMP file
file: SSY2K011.SA2_CJG_L464,

☒ Sensitivity set DIV file
file: PLEX_03MAY00_NG7.DIV,

☒ Absolute set ABS params
parameters: TSTAND=1;DSTAND=1;IZERO=1.130;

☒ Mask set MASK file
file: DEFAULT.MASK,

☒ Average set AVERAGE params
parameters: AVTYPE=Circular;SAVE=Yes;NAME=A

Save Protocol Export Reduce A File
Recall Protocol Import
Delete Protocol Done

Two additional items:

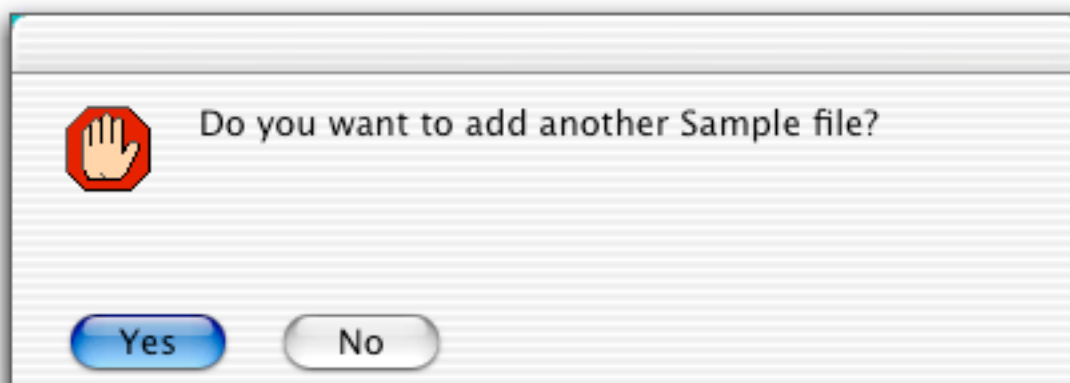
- Most experiments do not need to use a DRK correction file, which is measured with the main shutter closed. This measurement is typically only necessary when... just go ask your local contact if this correction is necessary for your experiment.

- Protocols can be "Exported" as a text file that can be "Imported" into a new reduction experiment. This is most useful for users with the Demo Version of IGOR, where a save of the whole experiment is not possible.

Reduce a File

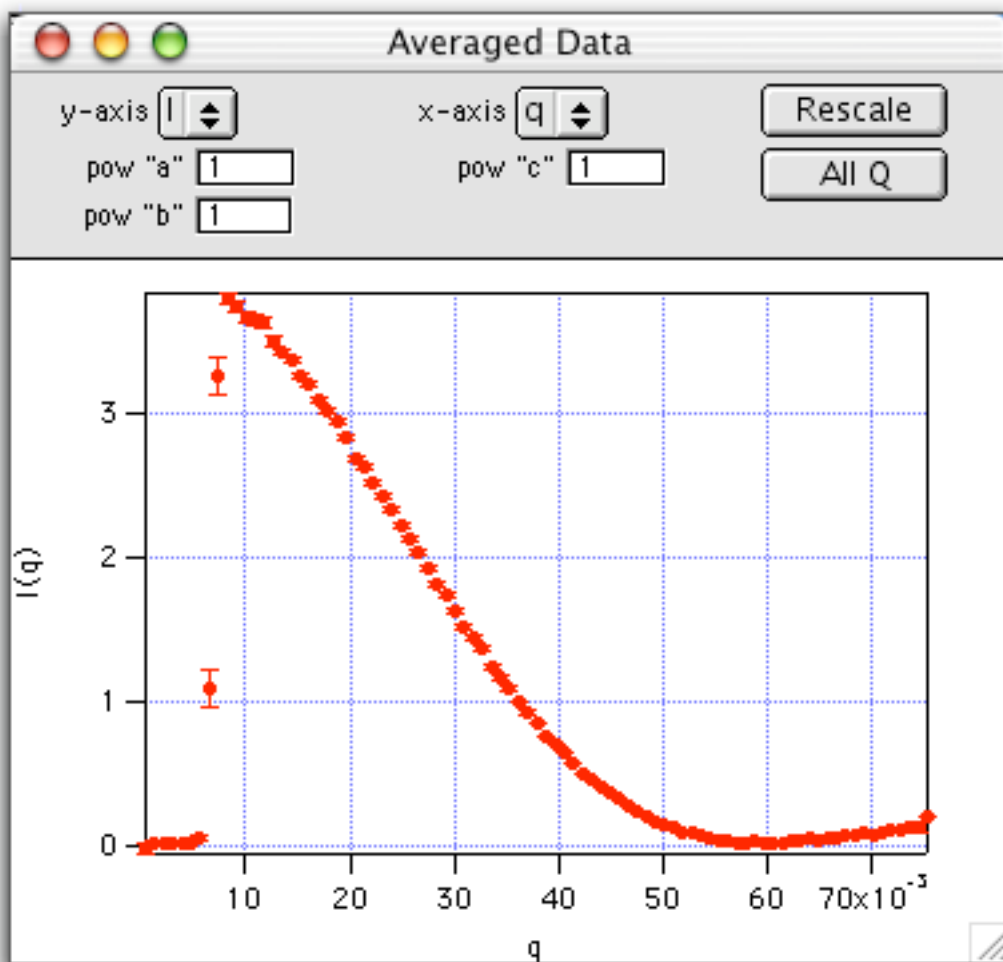
What: Process a raw SANS data file to a 1-D average using a previously saved protocol, or use a blank protocol where you will be prompted for each data file as needed.

How: Since we just created and saved our two protocols, we'll use them directly from the Protocol Panel. Start with the 6-meter protocol. To make sure it's in place, click "Recall Protocol" on the panel, and pick "sdd_6meter", or whatever you named it from the list. Your protocol choices are updated in the panel. At this point, you can choose the 6-meter apoferritin scattering file from the CAT/Short window, and "Set SAM File", or since the protocol says "ask", just let it prompt you with a file dialog. You could also enter a list of run numbers. When done, click "Reduce A File" on the Protocol Panel. Pick the scattering file from the dialog if prompted (it's run SSY2K004...). The file will be displayed, and you will be prompted to add another sample file, if desired:

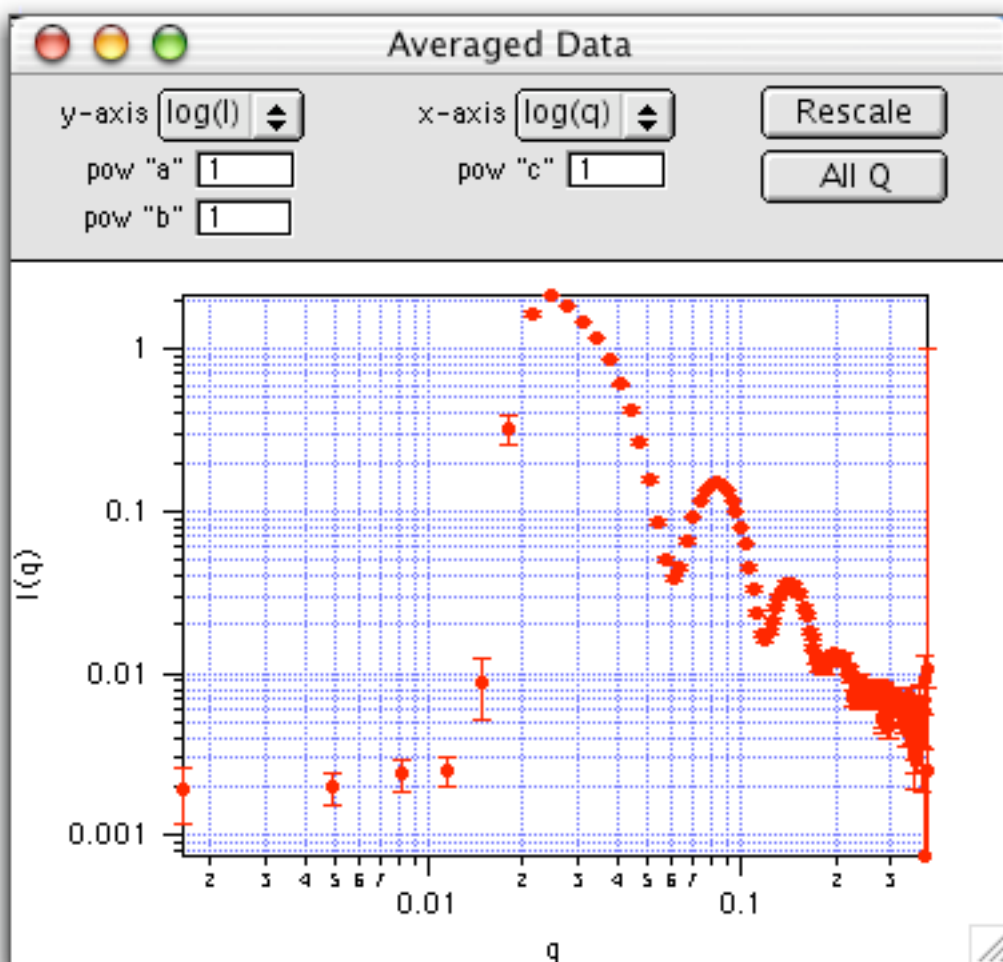


If you re-measure a sample at the identical configuration, you can add these raw data files together to improve the counting statistics. In this case, we only have one file, so (No) we don't want to add another data file.

The data reduction will proceed through the protocol, showing each intermediate step along the way. Watch closely - if something doesn't look right, go back and check it out after the reduction is done. If something is grossly in error, the reduction can be aborted (cmd-. on Macintosh, or the Abort button at the lower left in Windows). This example will proceed smoothly, of course. The final result should look like this, and the command window should indicate that a data file was written, and what filename was used.



Reduce the scattering data for the 1.6 meter configuration in the same way. "Recall" the protocol that you saved, and click "Reduce A File". You will be prompted for the sample scattering file (it's SSY2K009...) and the reduction will complete as before, using the files specified in the protocol. The final result for the high q data should look like this, once you've rescaled the X and Y-axes to log-scaling:



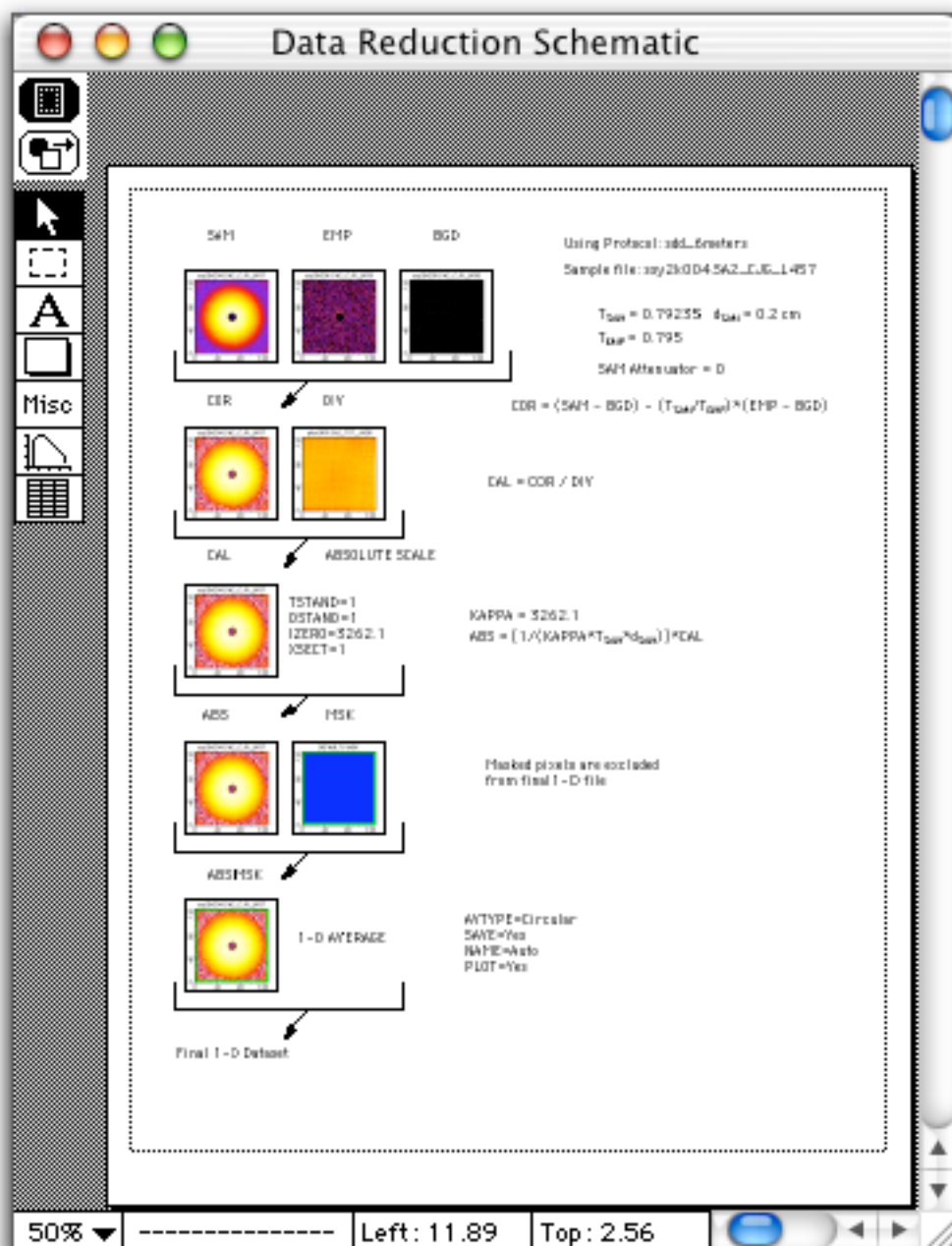
Instead of building a protocol, one could use either the "Base" protocol - which does only minimal corrections, or "DoAll" which will perform all of the data reduction steps. To see exactly which steps each of these would perform, "Recall" these blank protocols into the Protocol Panel. Unchecked steps in the protocol will be skipped, and "ask" will prompt you to pick the required files from a standard open file dialog.

Schematic of Data Reduction Operation

What: The Schematic operation reduces a data file using a previously saved protocol and creates a printable layout showing all the details. This helps you see what happened at each step of the way during the data reduction. It is very useful for diagnosing problems in data reduction. NOTE: if you are using a demo version of IGOR Pro, you will not be able to do this step (sorry), but you will be able to view the intermediate files individually, by using the "Display 2D" button on the [2-D Ops Tab](#) on the main panel.

How: To see what steps were used and what the files looked like, click "Show Schematic" on the Misc Ops tab of the main panel. You will be prompted for either log or linear scaling of the intensity data. Make your choice and click continue. You will then be prompted for the protocol. Choose one that you just created and saved. You will then be prompted for a "Sample Data file" - choose the appropriate scattering run again, and it will be reduced again in exactly the same way. Once the reduction is complete, small images of the

intermediate steps will be created, and placed in a layout window. This can be inspected (or printed in color) to see exactly what data files were used at each step, what numerical constants were used and what file was saved. A placeholder box titled "Not Used" is in place of steps that were not used (at your request) in the reduction protocol. A placeholder box titled "No Data" means that you wanted to use that step, but an error occurred, and no data could be found (usually a file has been improperly specified). The example below used log-scaling and the 6 meter apoferritin data set.



Reduce Multiple Files

What: In a typical SANS experiment, many scattering files are collected at the same instrument configuration, and must be reduced using the same protocol. This operation allows

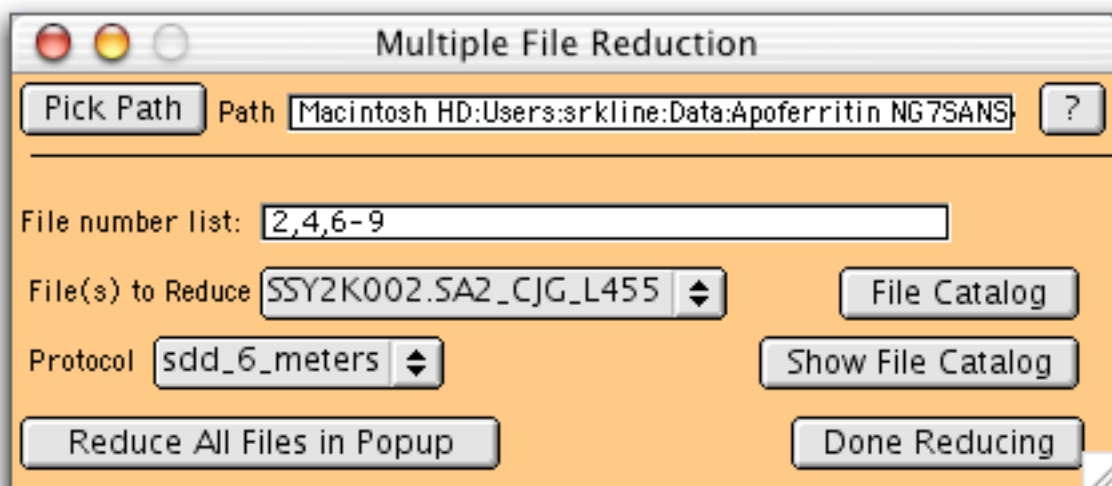
you to reduce SANS data in a batch mode using a previously saved protocol.

How: Since this tutorial only works with one file at each instrument configuration, no data will actually be processed here. Click "Reduce Multiple Files" on the Data Reduction tab of the Main Panel. This will display a new panel with a simple interface, used as follows:

1) Enter a comma-delimited list of run numbers to be reduced (leading zeros are not needed). Note that a 'dash' can be used to indicate an inclusive range of file numbers. Hit enter or return when finished, and this list of raw data files will be displayed in the popup list. If any of the data files cannot be found, you will be alerted to the offending file number. Check the popup list to confirm that these are indeed the file(s) that you want to reduce.

2) Select the appropriate protocol from the popup (you must have already created / tested / saved it from the Protocol Panel) to be used to reduce the selected files.

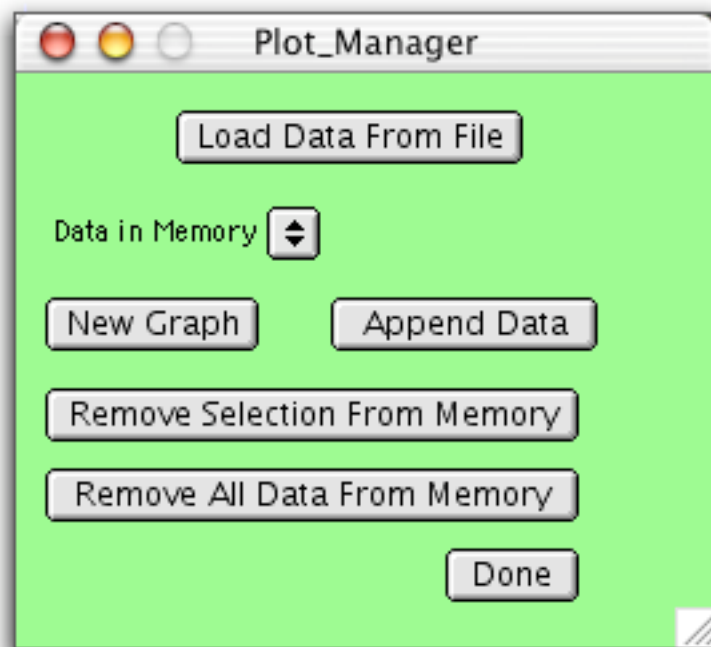
3) At this point you would click "Reduce All in Popup" to reduce all of the files in the list with the chosen protocol. Of course, don't do it with the tutorial data - the files in the list are not all at the same configuration - it's just an example. As each file is reduced, all of the intermediate steps are shown. Automatic naming is the best choice in a protocol when reducing multiple files, since no input is required from the user.



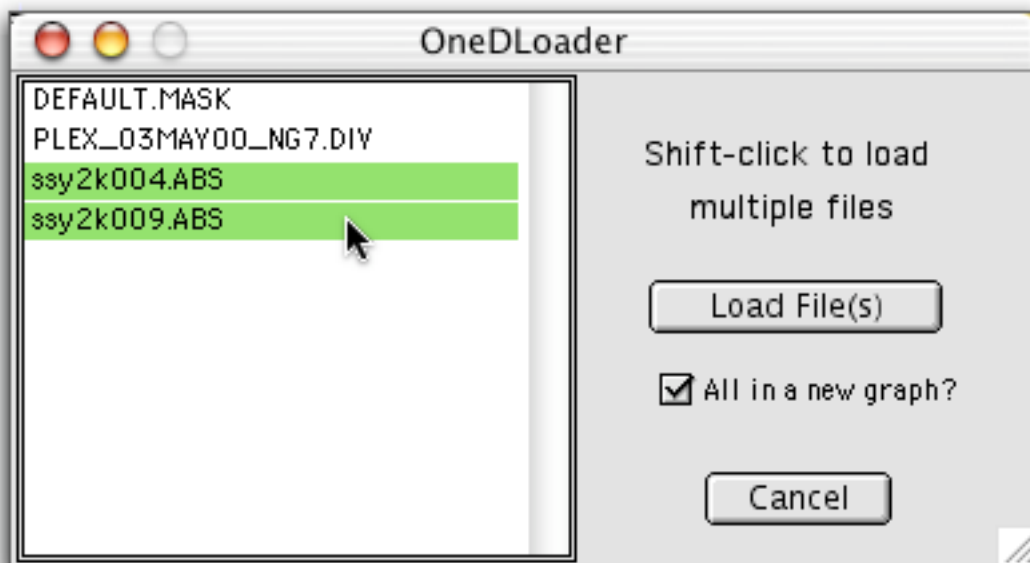
Plot Averaged Data

What: Plots 1-D averaged data files in a nice graph, allowing you to plot multiple datasets on the same graph.

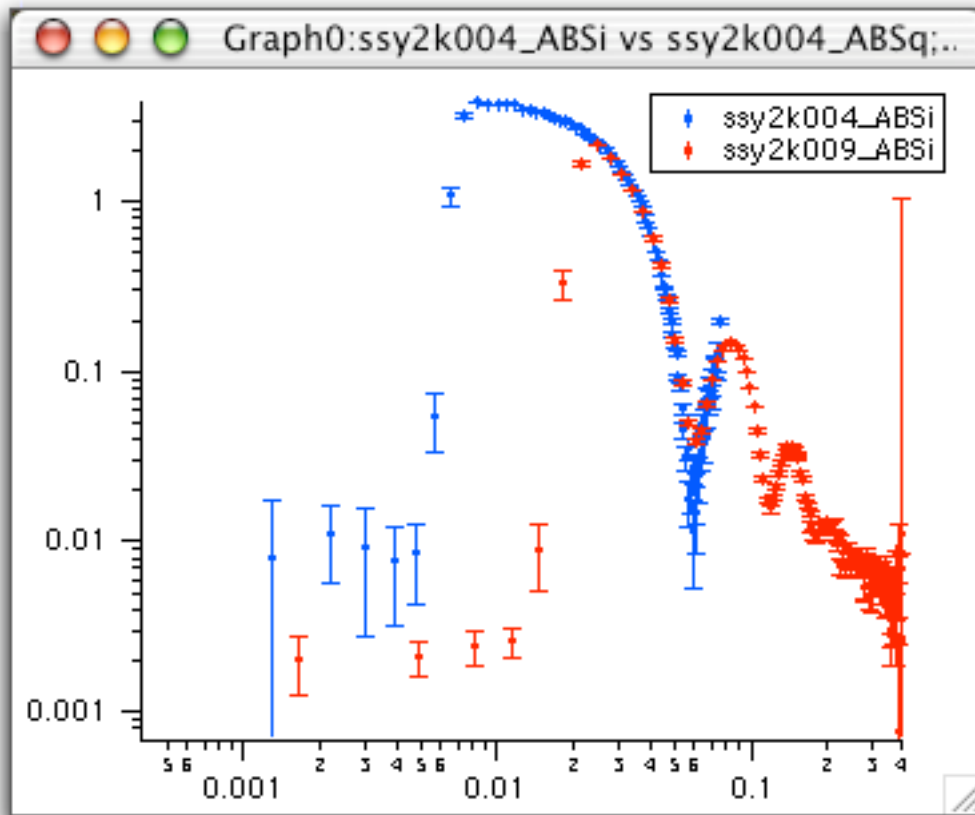
How: Click "Plot" on the 1-D Ops tab on the main panel, and the Plot Manager panel will appear.



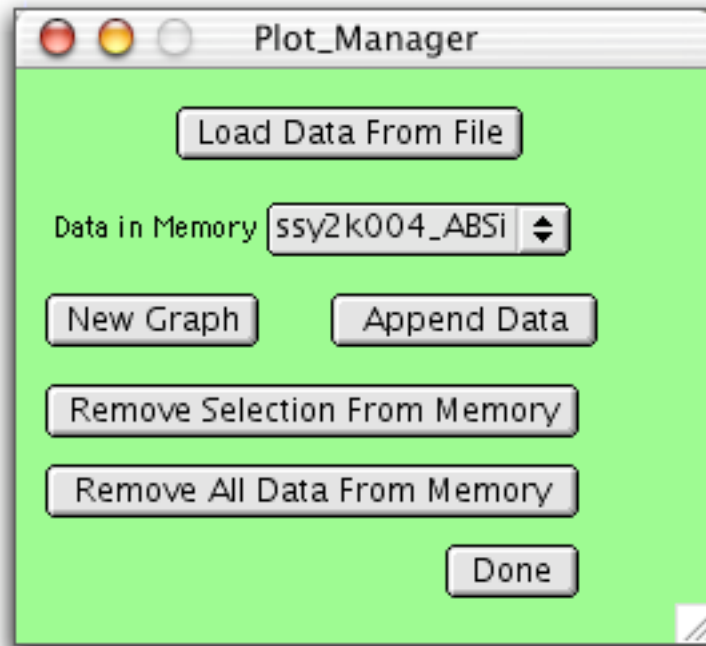
Initially, there is no data loaded in memory, so use "Load Data From File" to load and plot the data from both detector distances, files SSY2K004.ABS and SSY2K009.ABS. The listing of data files is from the same data path that you set from the Main Panel. Note that there may be some files in the list that are not 1-D averaged data.



Leave the checkbox selected to automatically graph all of the selected files on the same, new graph. Shift-click to select both data files, then "Load Files" to load and graph both data sets on the same plot:

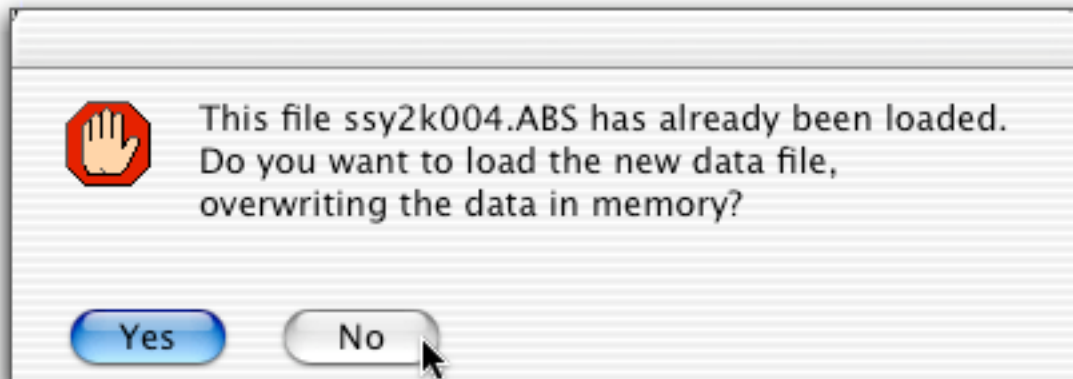


If you don't want all the data on the same graph, uncheck the box, and you will be able to graph and append data as you choose from the Plot Manager Panel. "New Graph" will create a new graph using the data set selected in the popup menu. "Append Data" will do just that to the topmost graph. Unwanted data files in the popup list can be removed from memory (the data on disk is NOT removed!) by either removing the selected file, or all files. Any data that is "in use" in a table or a graph won't be removed, and will remain in the popup list. You will have to close (and Kill) any open graphs to then be able to remove the data from memory.



NOTES:

- If you try to load a data set that is already in memory, you will see the dialog below. Clicking yes will load a fresh copy from disk into IGOR's memory. Clicking no will leave the data in memory unchanged. If you know that the data sets are the same, there is no harm in overwriting the data set in memory.



- To change the graph appearance, click on what you want to change, and a dialog will appear. The Graph menu also allows for a wide variety of customization of the graph appearance.
- The 2-D Display window is also a graph. If the Display window is on top, you don't want to overlay a 1-D dataset on top. If you do, the display will look garbled - just close the 2-D display and it will redisplay correctly the next time it is drawn.

Sort and Combine Averaged Datasets

What: After collecting data at 2 or 3 instrument configurations, it is convenient to combine these data files into a single file, eliminate "bad" data points, and scale the data sets to overlap. Plot the individual data files at the two different q-ranges, trim off the "bad" data points (behind the beamstop and at the corners of the detector), automatically adjust the scaling to get perfect overlap between datasets, and write out the combined data file. In addition, a single data set can be trimmed and rescaled

How: Click "Sort" on the 1-D Ops tab on the Main Panel. This will display a new panel.

NSORT_Panel

NSORT - Rescale and combine 1-D files

Pick Path Path: Macintosh HD:Users:srkline:Data:Apoferrit ?

Low Q: Delete Points? Plot

DEFAULT.MASK Beg Pts 0 End Pts 0

☒ Normalize to this file

Medium Q: Delete Points? Plot

none Beg Pts 0 End Pts 0

☐ Normalize to this file

High Q: (or none) Delete Points? Plot

none Beg Pts 0 End Pts 0

☐ Normalize to this file

☒ Auto Scale Mult factor 1-2 1 Mult factor 2-3 1

To Manually scale data, enter scale factors above

Write Combined File Done

Select the data set with the lowest q-values (the 6-meter data set, ssy2k004.abs) as the "Low Q" data file. Plot it, and remove points from the beginning and end of the set that were behind the beamstop or at the edges with large error bars (the omitted points will be displayed as open circles, and are a copy of the original data set). Do the same for the higher q-range (the 1.6-meter set) as the "Medium Q" dataset. If you had a third, still higher q-range, you would plot that set as "High Q", but we have none. Note that if you only have data from two

instrument configurations, treat them as "Low" and "Medium" and set the "High Q" set to "none". If you have only one data set, it is the "Low Q" set, and both Medium and High Q popups should be set to "none".

NSORT_Panel

NSORT - Rescale and combine 1-D files

Pick Path Path: Macintosh HD:Users:srkline:Data:Apoferri ?

Low Q:

ssy2k004.ABS

☒ Normalize to this file

Delete Points?

Beg Pts 10

End Pts 5

Plot

Medium Q:

ssy2k009.ABS

☐ Normalize to this file

Delete Points?

Beg Pts 19

End Pts 10

Plot

High Q: (or none)

none

☐ Normalize to this file

Delete Points?

Beg Pts 0

End Pts 0

Plot

☒ Auto Scale

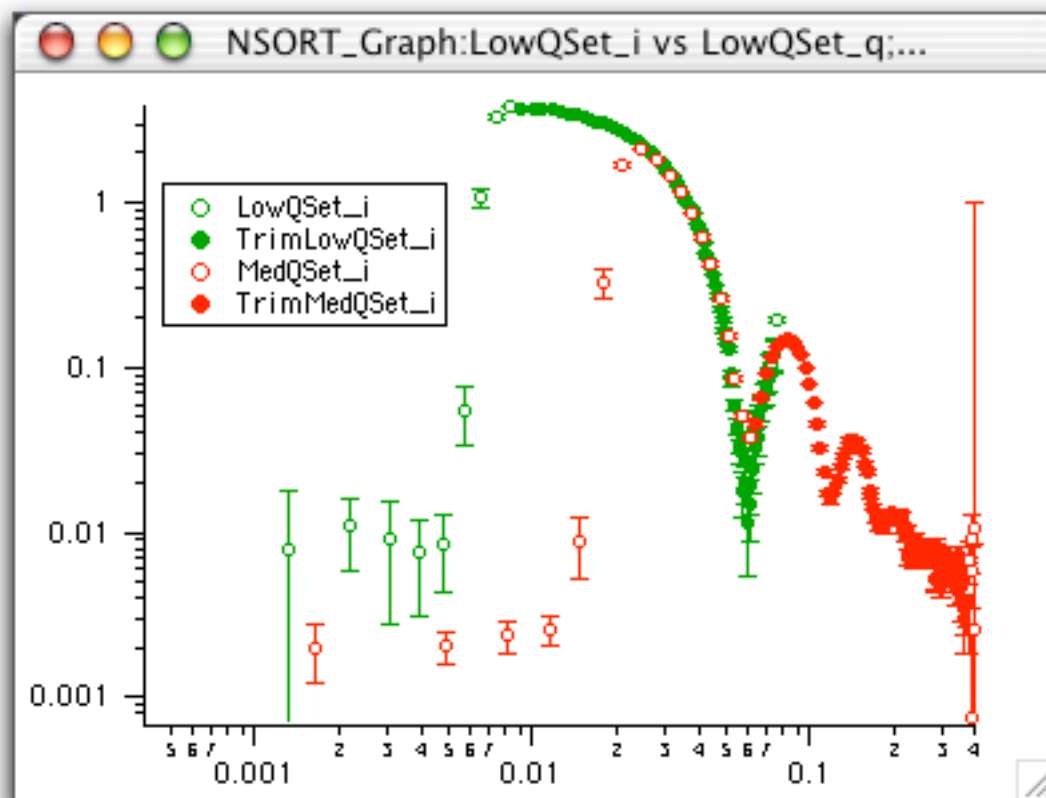
Mult factor 1-2 1

Mult factor 2-3 1

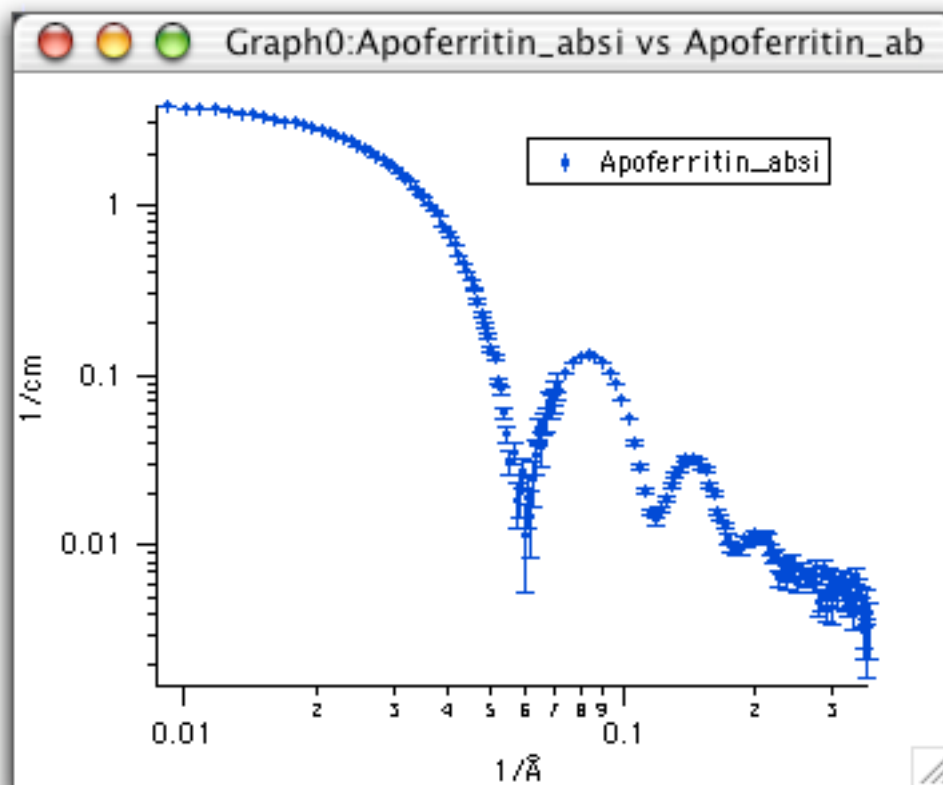
To Manually scale data, enter scale factors above

Write Combined File Done

The NSORT graph should look something like this. Be sure "auto scale" is selected for automatic calculation of the overlap constant (or you can enter your own if you wish). Also check the set that you want the combined set to be normalized relative to (you can only choose one). Click "Write Combined File" to create a new file. You will always be prompted for a new name for the combined data set. The header of this file will indicate which files were combined, and the scaling factors used. The automatic scale factor(s) are reported to the panel. For datasets already on absolute scale, the scaling factor should not be far from unity.



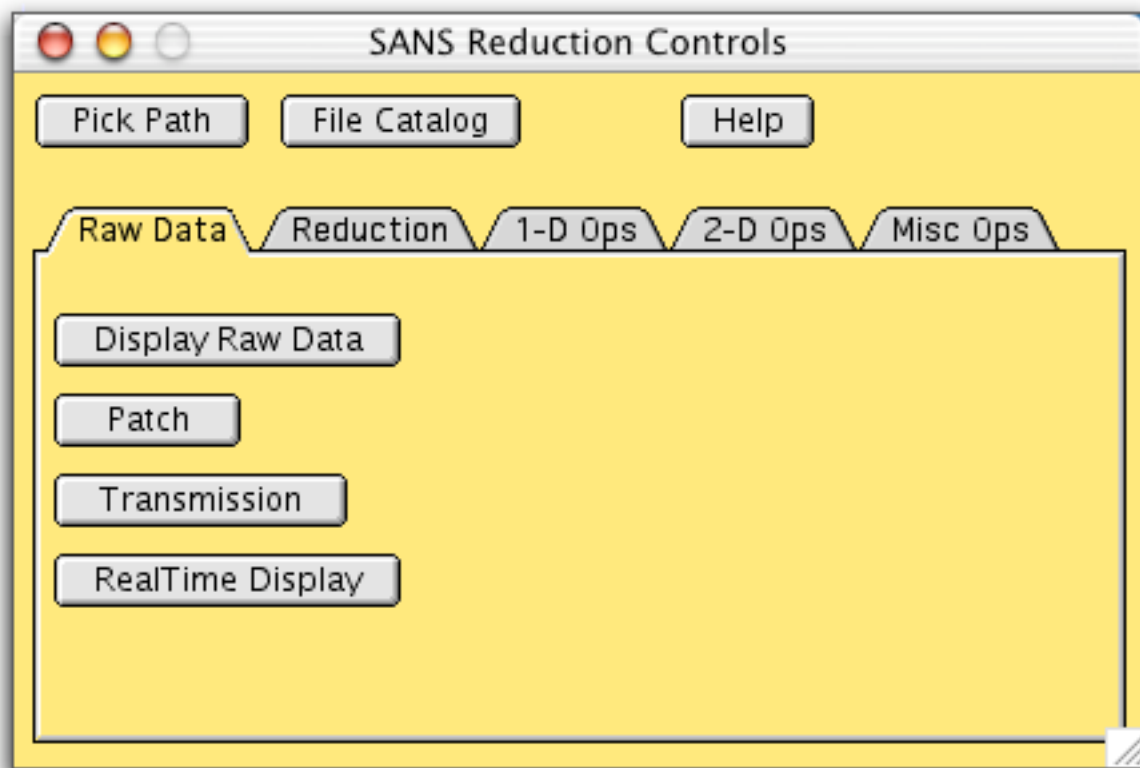
The final, combined and overlapped dataset (I named it Apoferritin.abs), once plotted should look something like this:



Additional Operations

Main Panel Tabs

Raw Data Tab



The buttons are:

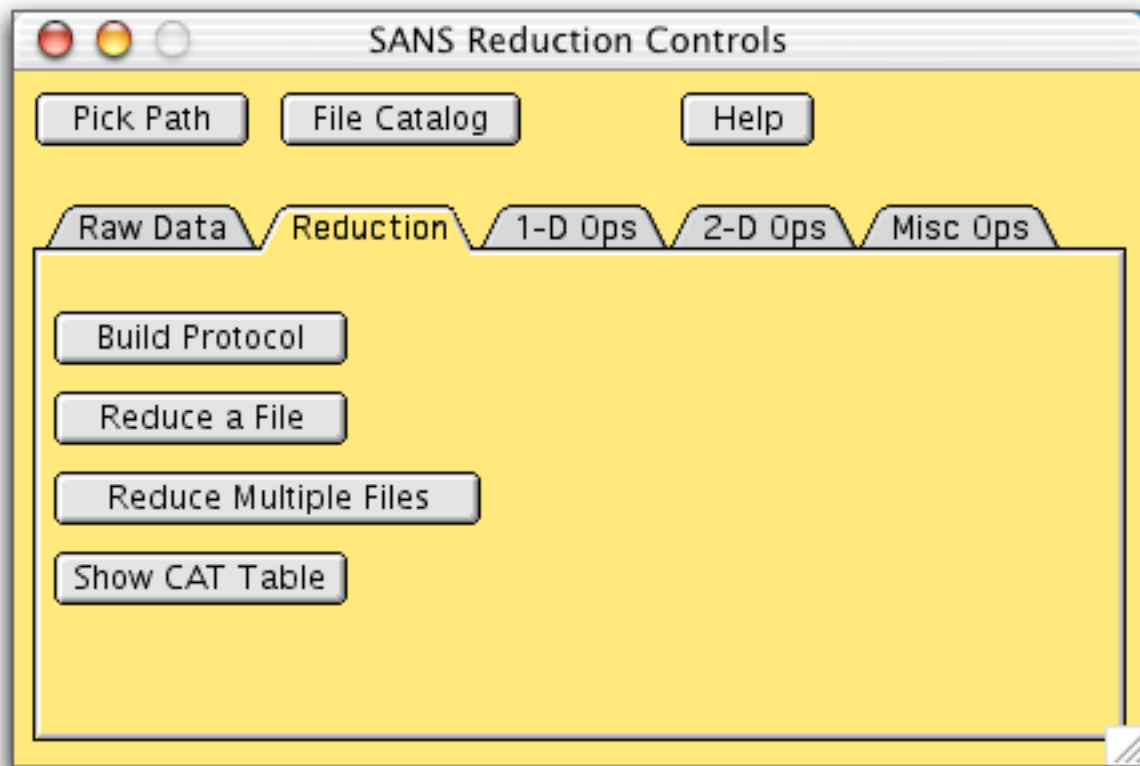
Display Raw Data: presents an open file dialog to select a raw SANS data file for display, then graphs it as a 2-D image with lots of helpful information.

Patch: generates a separate panel where you can change a selected number of parameters that are stored in the header of the raw (binary) SANS data files.

Transmission: generates a separate panel with controls to allow you to set the relations between transmission files and scattering files, then to finally calculate the sample transmissions.

RealTime Display: generates a separate panel with controls for display of the live detector image. This operation is only useful during data collection at the NG1 SANS instrument at NIST.

Reduction Tab



The buttons are:

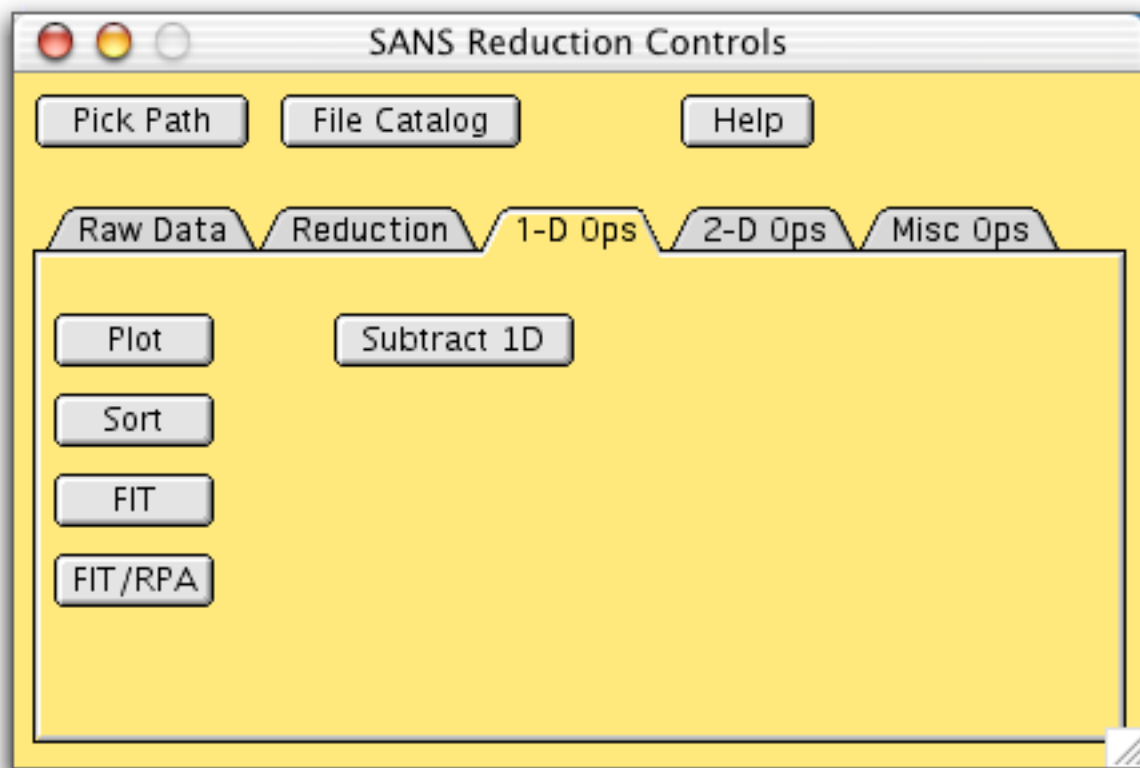
Build Protocol: generates a separate panel with controls to allow you to sequentially build the desired steps of a reduction protocol. The File Catalog table is used interactively to build protocols, so have the table handy.

Reduce A File: will prompt you to select a protocol, then for a sample file, followed by each of the reduction steps specified by the protocol.

Reduce Multiple Files: generates a separate panel with controls to allow you to reduce files in batch mode, using a protocol that you have previously created and saved using the Build Protocol panel.

Show CAT Table: simply brings the File Catalog table to the front, if it is open. It does not re-build the table from a directory listing.

1-D Ops Tab



The buttons are:

Plot: presents an open file dialog to select an averaged (1-D) dataset, and then graphs it. Multiple datasets can be plotted on a single graph.

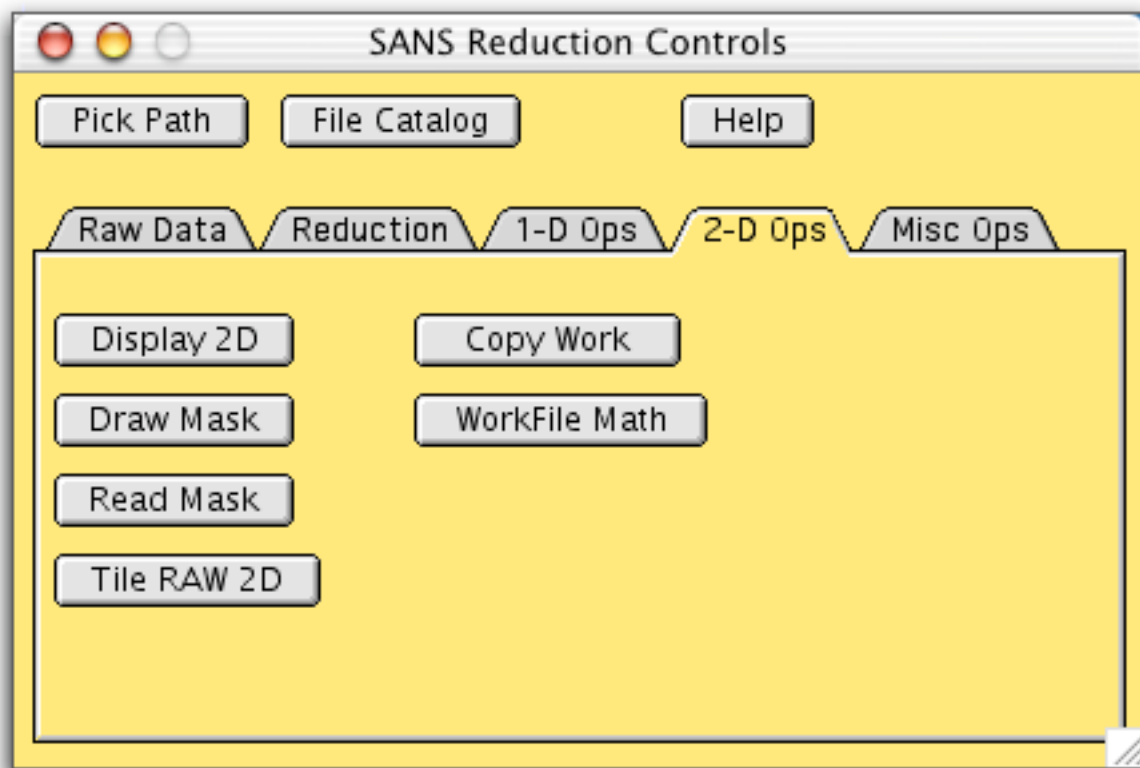
Sort: generates a separate panel with controls to sort, internormalize, delete "bad" points, and finally combine averaged datasets from different instrument configurations into a single file.

Fit: generates a separate panel with controls to perform linearized fits to 1-D datasets. Fits can be interactively refined. Often used during the reduction of secondary intensity calibration standards.

Fit/RPA: generates a separate panel with controls to perform an RPA fit to 1-D data generated from a polymer sample used as a secondary intensity standard.

Subtract 1D: generates a separate panel with controls to perform subtractions of 1D data sets. Very useful for subtracting buffer scattering from sample scattering, and for subtraction of a constant background value.

2-D Ops Tab



The buttons are:

Display 2D: presents a dialog to select and display one of the intermediate work file types.

Draw Mask: generates a separate graph (of the currently displayed 2-D dataset) with controls to draw and save a mask to eliminate "bad" detector pixels from the final averaged (1-D) dataset.

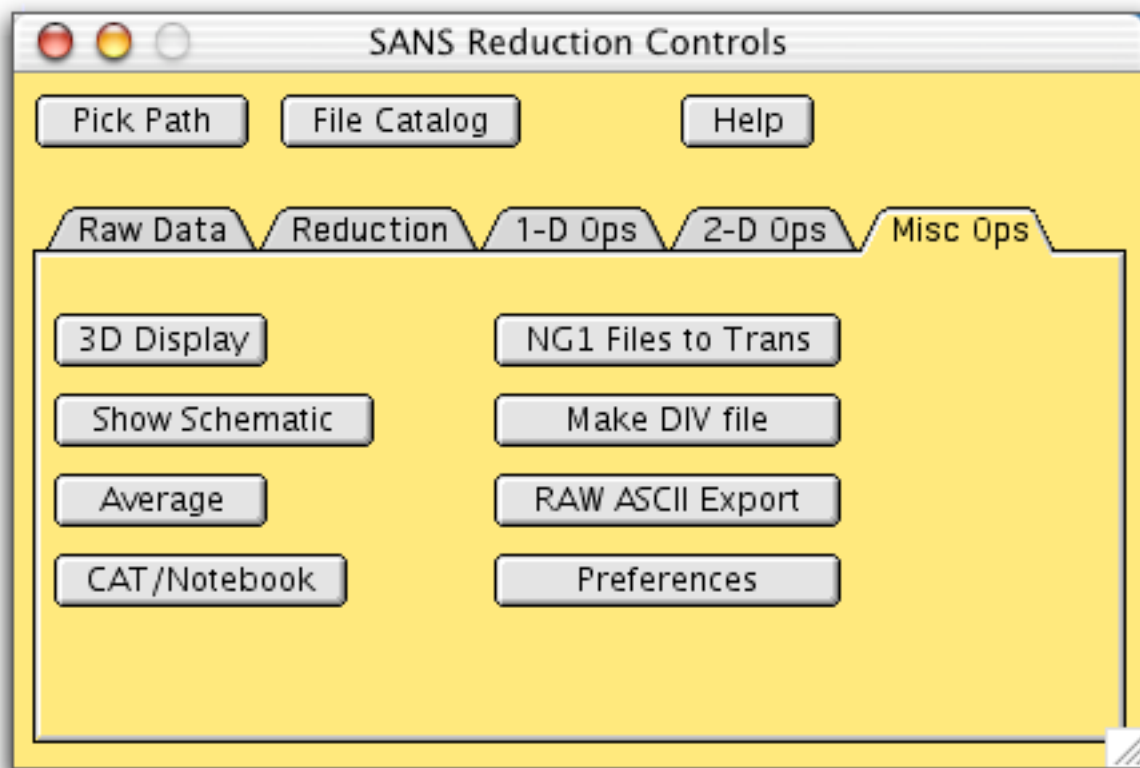
Read Mask: presents an open file dialog to read in a previously saved mask file and generates a small image of the mask.

Tile RAW 2D: generates a separate panel with controls to select any number of raw SANS files, then append images of these files to a Layout window. Images can be arranged in the layout, annotated, and printed.

Copy Work: copies the entire contents of a selected folder to a target folder.

WorkFile Math: generates a separate panel with controls to perform simple arithmetic operations on two (2-D) ASCII files that have been previously saved.

Misc Ops Tab



The buttons are:

3D Display: displays the selected work file type as a 3-D wireframe plot.

Show Schematic: generates a layout showing all of the intermediate steps and files used during the reduction of a selected file and its protocol. Very useful for diagnosing data reduction errors.

Average: presents the panel with 1-D averaging options, to be applied to the currently displayed data.

CAT/Notebook: generates a notebook with information about each file in the selected data path. Somewhat less information than File Catalog, but in a notebook (text) format.

NG1 Files to Trans: generates a separate panel with controls to convert RAW transmission data files collected at NG1 SANS into raw data files that can be interpreted as such during transmission calculation.

Make DIV File: to be used only by NIST instrument scientists to generate detector sensitivity files for general use.

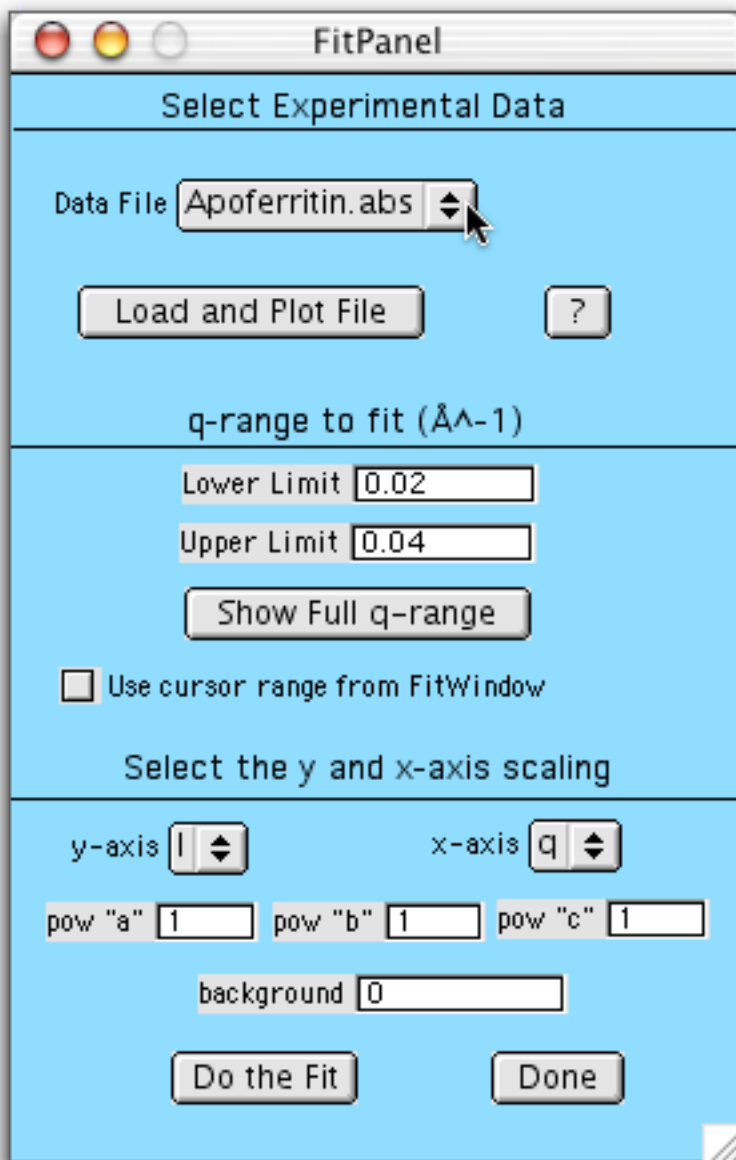
RAW ASCII Export: generates a separate panel with controls to export selected RAW SANS data files in ASCII format, either as detector pixels, or in I(Qx,Qy) triples.

Preferences: generates a separate panel used to set several specific parameters as desired by the user. Running "Initialize" from the SANS menu will return values to their default state.

Fit Lines to Your Data

What: To obtain some quantitative information about your sample, a variety of linearized fits can be performed such as: Guinier fits, Zimm plots, Kratky plots, power laws, and other forms. Linearized fits are also used to extract absolute scaling parameters from secondary standards (Al-7, water, silica A/B).

How: The reduced data file Apoferritin.abs is scattering from some sort of protein, and appears to have a Guinier region at low q . From the 1-D Ops tab on the Main Panel, click "FIT". The following panel will appear.

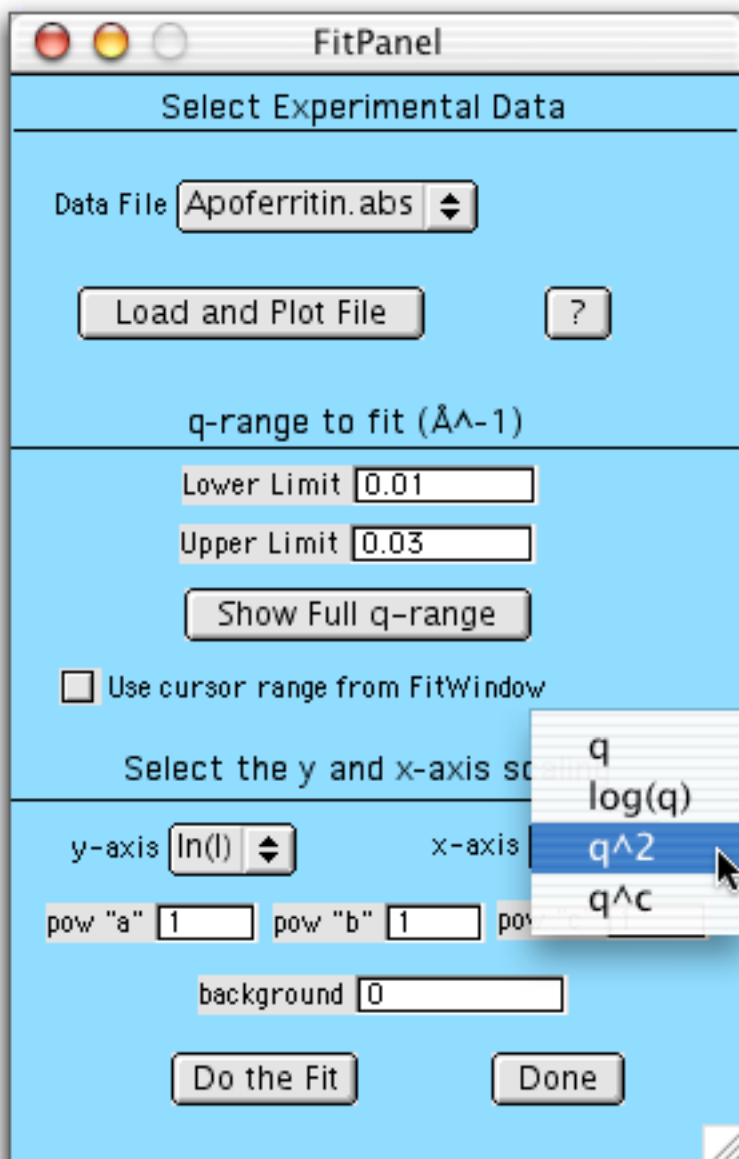


The image shows a software dialog box titled "FitPanel". It has a light blue background and a standard Mac OS window header with red, yellow, and green buttons. The dialog is organized into several sections:

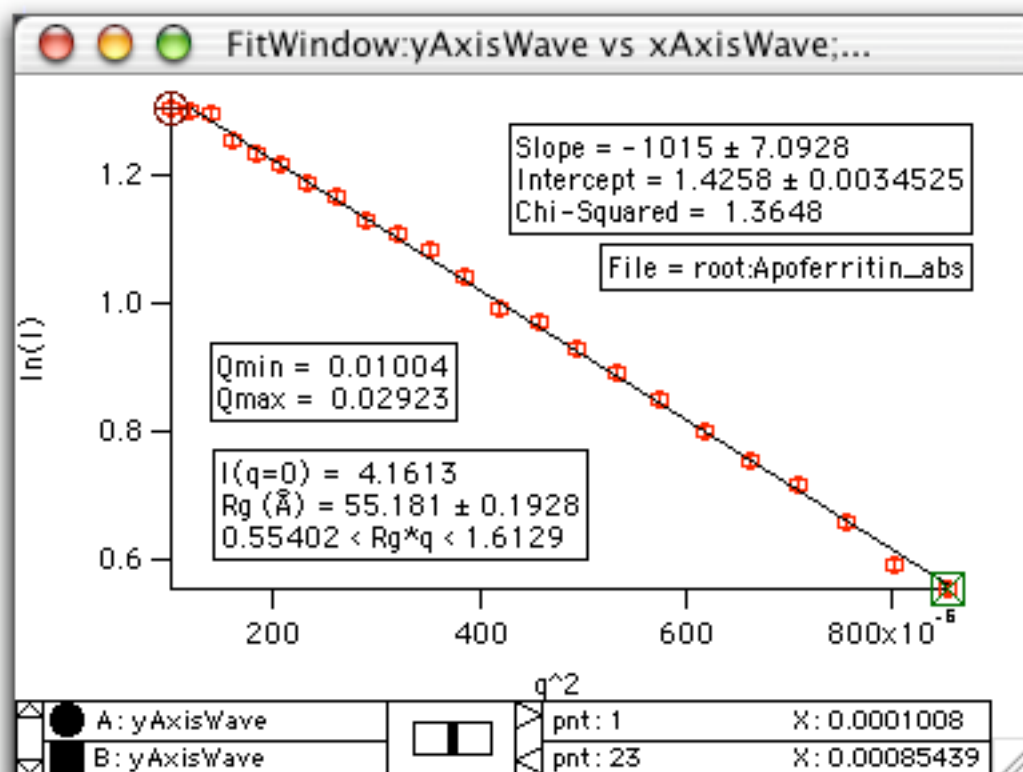
- Select Experimental Data:** Contains a "Data File" dropdown menu with "Apoferritin.abs" selected. Below it are two buttons: "Load and Plot File" and a help button with a question mark.
- q-range to fit (\AA^{-1}):** Contains two input fields: "Lower Limit" with the value "0.02" and "Upper Limit" with the value "0.04". Below these is a button labeled "Show Full q-range".
- Use cursor range from FitWindow:** A checkbox that is currently unchecked.
- Select the y and x-axis scaling:** Contains two dropdown menus: "y-axis" with "I" selected and "x-axis" with "q" selected. Below these are three input fields for powers: "pow 'a'" with "1", "pow 'b'" with "1", and "pow 'c'" with "1".
- background:** An input field with the value "0".
- Buttons:** At the bottom are two buttons: "Do the Fit" and "Done".

Choose the apoferritin.abs data file in the first popup list. We want to fit this data over the range (0.01 - 0.03) [$1/\text{\AA}$]. Enter these values if they are not already there. To fit the data to a Guinier plot, select a y-axis scaling of " $\ln(I)$ " and an x-axis scaling of " q^2 ". The powers a, b, and c apply to different axis scalings, and we do not need to subtract any

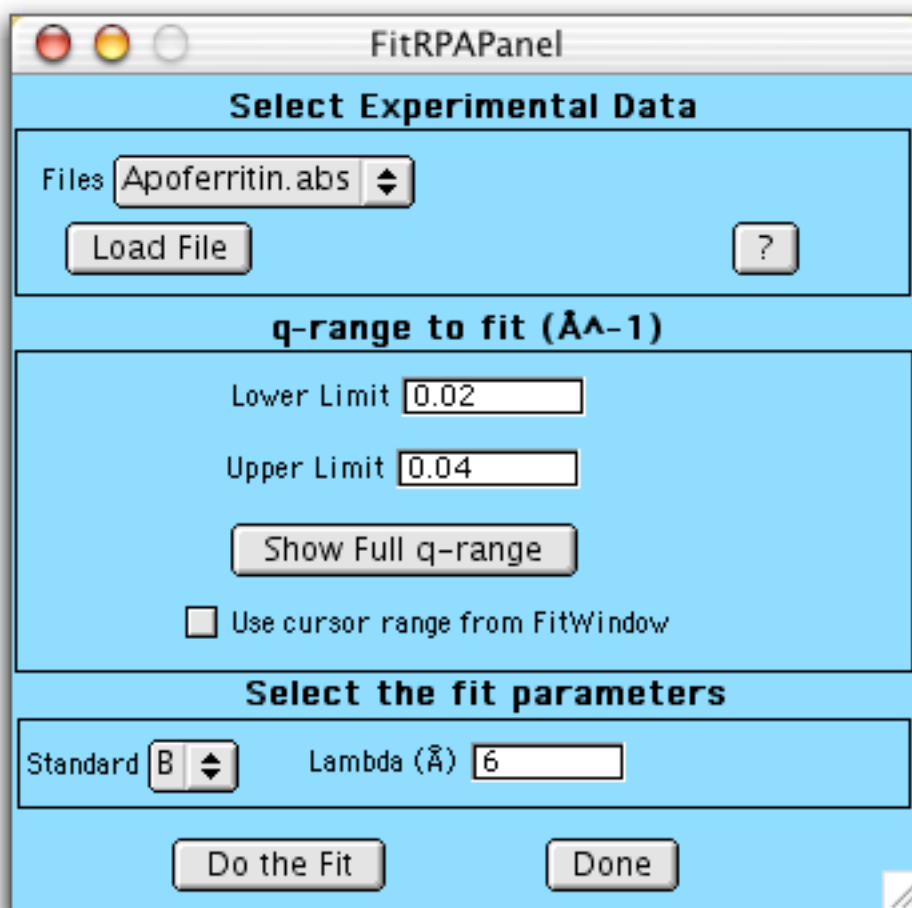
background before doing the fit. Click "Do the Fit", and the data is scaled and fitted, with all the statistics on the graph. One standard deviation is reported along with the radius of gyration and range of $q \cdot R_g$.



This looks like a good fit, but the fit can be adjusted by either entering new q -values, moving the cursors on the graph to "better" data points, or subtracting a background value before the linearized fit is performed. Clicking "Show Full q -range" does just as stated. The data range that was fitted is marked by the cursors (and is hopefully linear for a Guinier plot).



The secondary polymer standards are fitted with an RPA model (Random Phase Approximation) in order to extract the absolute scaling parameters. This panel "Fit/RPA", also from the 1-D Ops tab on the main panel, behaves much like the FIT panel. The model is specific for the polymer standards, so you need to be sure to choose the proper standard.



The image shows a software window titled "FitRPAPanel". It has a light blue background and a white title bar with standard Mac OS window controls (red, yellow, and green buttons). The window is divided into three main sections. The first section, "Select Experimental Data", contains a "Files" dropdown menu with "Apoferritin.abs" selected, a "Load File" button, and a question mark button. The second section, "q-range to fit (\AA^{-1})", contains input fields for "Lower Limit" (0.02) and "Upper Limit" (0.04), a "Show Full q-range" button, and a checkbox labeled "Use cursor range from FitWindow" which is currently unchecked. The third section, "Select the fit parameters", contains a "Standard" dropdown menu with "B" selected and a "Lambda (\AA)" input field with "6" entered. At the bottom of the window are two buttons: "Do the Fit" and "Done".

Subtract 1D Data

What: Subtract two 1D data files (.ABS or .AVE) or rescale a single file. Most useful for subtracting a solvent "blank" from the sample + solvent scattering. Often this can be done more accurately after both files have been reduced to 1D data sets. A constant (q-independent) background can also be subtracted from a single data set.

How: Reduce your data to 1D ASCII files, sort and combine to get data sets that are free from data points obscured by the beamstop and excessively noisy data at the detector edges. From the 1-D Ops tab on the Main Panel, click "Subtract 1D". The following panel will appear as well as an empty graph. No sample or solvent data has been specified, so click on "Load Sample" to load in the Apoferritin data.

Solvent Subtraction

Sample Scattering File: : <none>

☐ Rescale Sample file? **Load Sample** ?

Solvent Scattering File: : <none>

Load Solvent

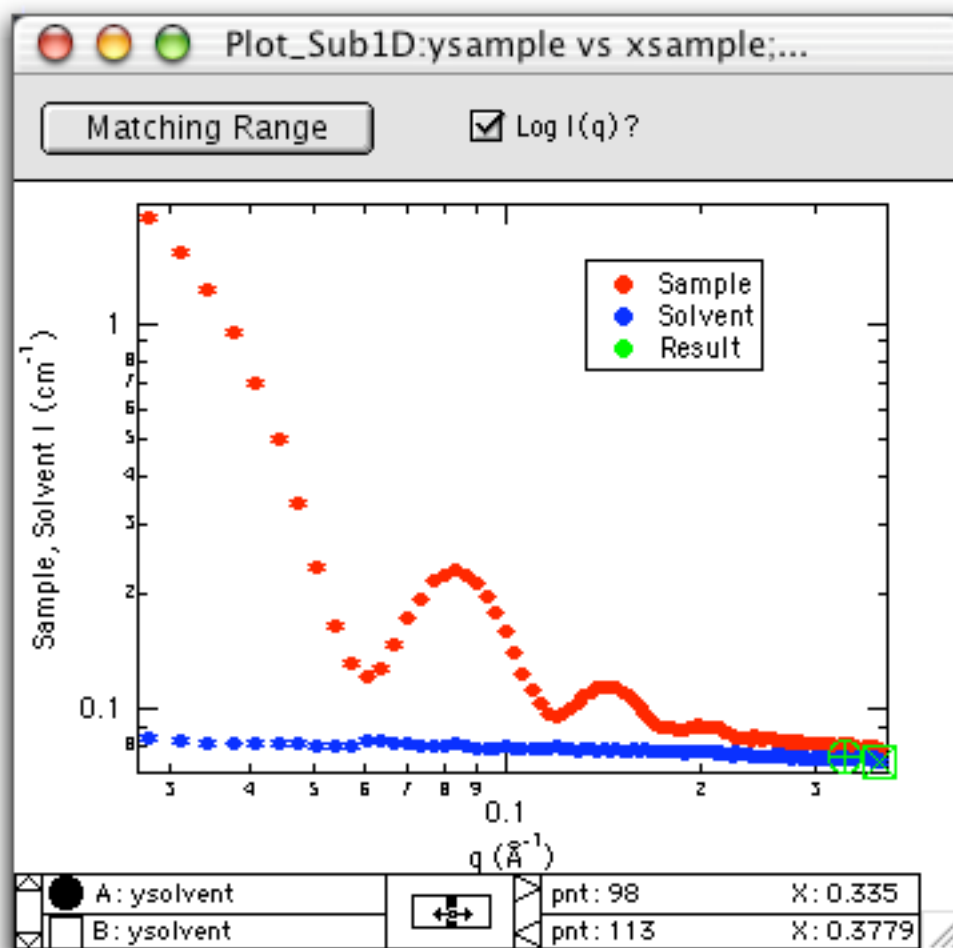
Result: $I = I - f * I$ ☐ Solvent = 1?

Matching Range Start: 0 ☐ Preset f manually?

End: 0 f : 1

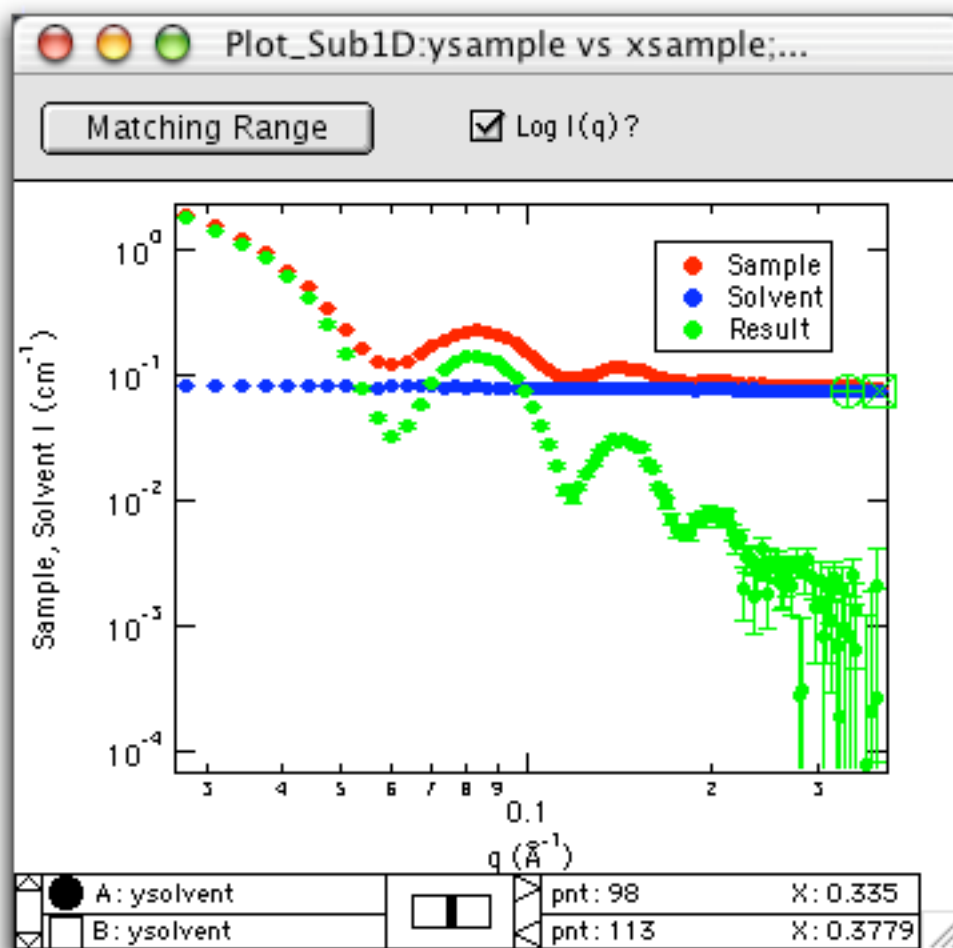
Calculate **Save Result** **Done**

For this example, I created reduction protocols that subtracted only the blocked beam component from the sample scattering, and treated the apoferritin and the buffer as separate "samples". The following graph shows the apoferritin (with buffer) data and the buffer data, loaded as the "Solvent Scattering File".



The cursors on the graph are both on the solvent data set. Adjust the cursors to move them to the high q end of the solvent scattering data set. The data range defined between the cursors will be the "Matching Range" where the subtraction will be scaled (by the factor "F" in the panel) such that the result has an average value of zero in that range. Click on the "Matching Range" button either on the graph or on the panel, they're both the same. The starting and ending q -values will appear in the panel. Note that you can zoom in on the graph by clicking and dragging a rectangular region on the graph (say around the cursors) and then click inside the marquee to get a contextual menu, and select "Expand". To see the whole axis range again, type CMD-A (Mac) or ctrl-A (Win).

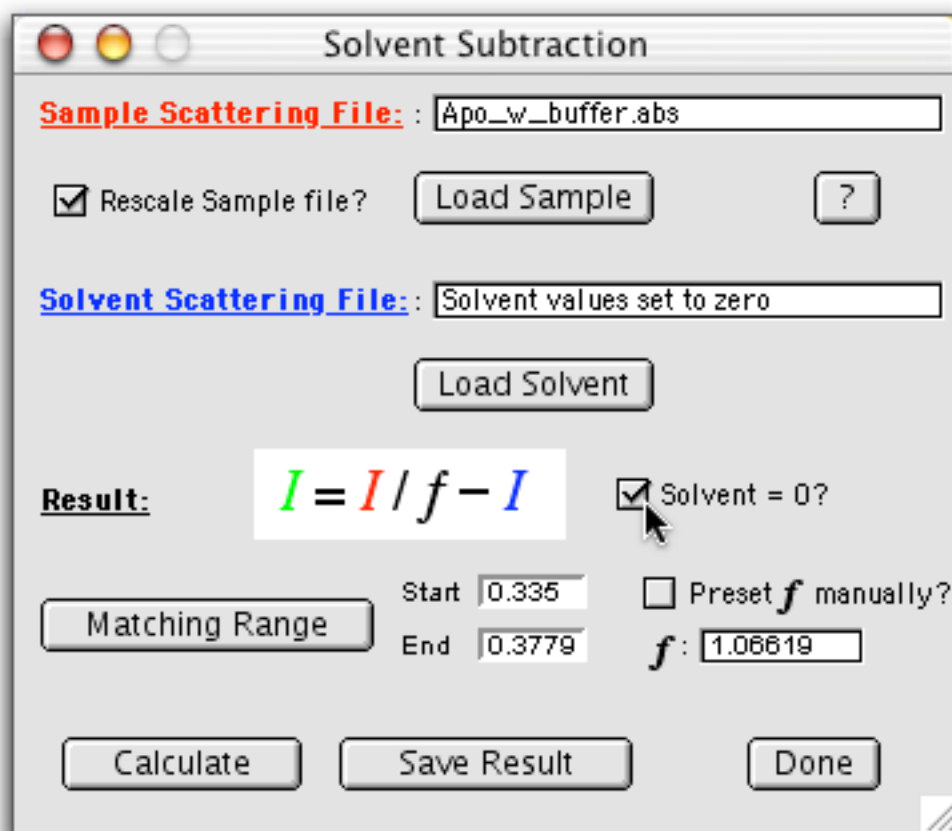
Once you've set the cursors to an appropriate range, and clicked to set the "Matching Range", click "Calculate" on the panel. The result (in green) should appear something like this, and should look very close to the original apoferritin data set that had the buffer scattering subtracted at the 2D level:



The matching range can be further adjusted, or the fraction of solvent subtraction can be set manually to fine-tune the subtraction. At this point, the resulting subtraction can be saved, using "Save Result".

A constant (Q-independent) background can be subtracted by loading a sample file, and checking the box "Solvent = 1?" for the solvent data ($l = 1$ in the equation). Then the matching range is set as before, and this scaled (constant) value is subtracted. The constant to subtract can also be set manually.

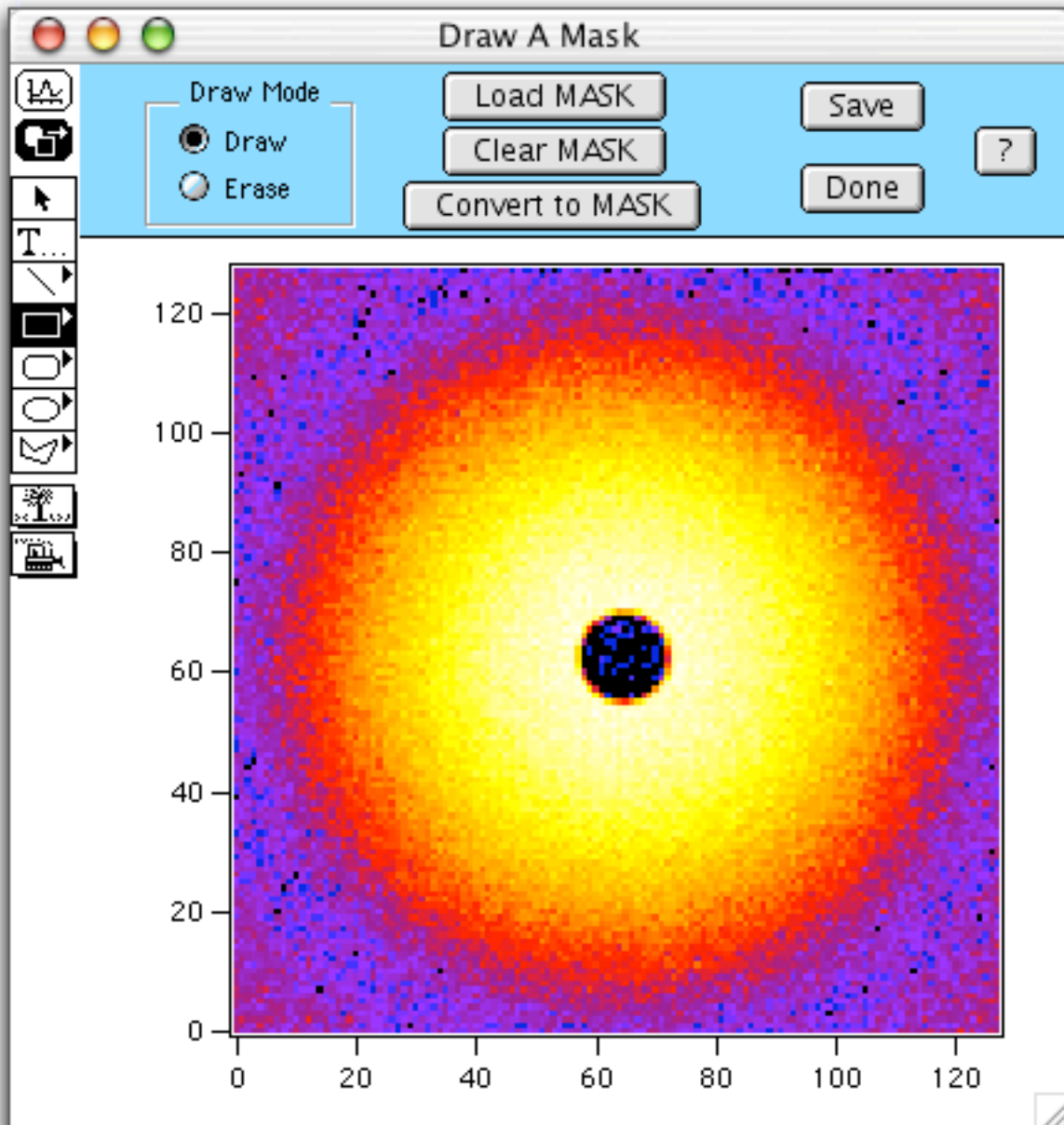
Checking "Rescale Sample File" changes the formula for the calculation of the result, allowing rescaling of the sample data set and subtraction of a solvent file. This solvent file can be set to zero if desired. In this "rescaling" mode, the scaling factor in the Matching Range is chosen to make the average value in that range equal to one.



Draw a Mask

What: The edges of the detector, typically 1 or 2 channels, do not count as reliably as the remainder of the detector, and should not be averaged into 1-D data. This is the usual case, and the "default.mask" should be used. Occasionally, localized regions of the detector image may need to be masked. Then a custom mask must be drawn, so that the MASKed pixels will be ignored during the averaging step.

How: Display a representative raw data file, then click "Draw Mask" on the main panel. The following window appears.



The control bar allows:

Draw and Erase: modes are set by the radio buttons. In Draw mode, draw objects are added to the mask file. In Erase mode, draw objects are erased from the mask.

Load Mask: loads a specified mask and puts it into the current draw layer, allowing you to "edit" a previously created mask file.

Clear Mask: clears ALL of the mask that is currently being drawn, giving you a clean slate to work from.

Convert to Mask: takes the current draw objects and converts them to the current mask (cumulatively), drawing or erasing pixels depending on the mode setting **when the objects were drawn**.

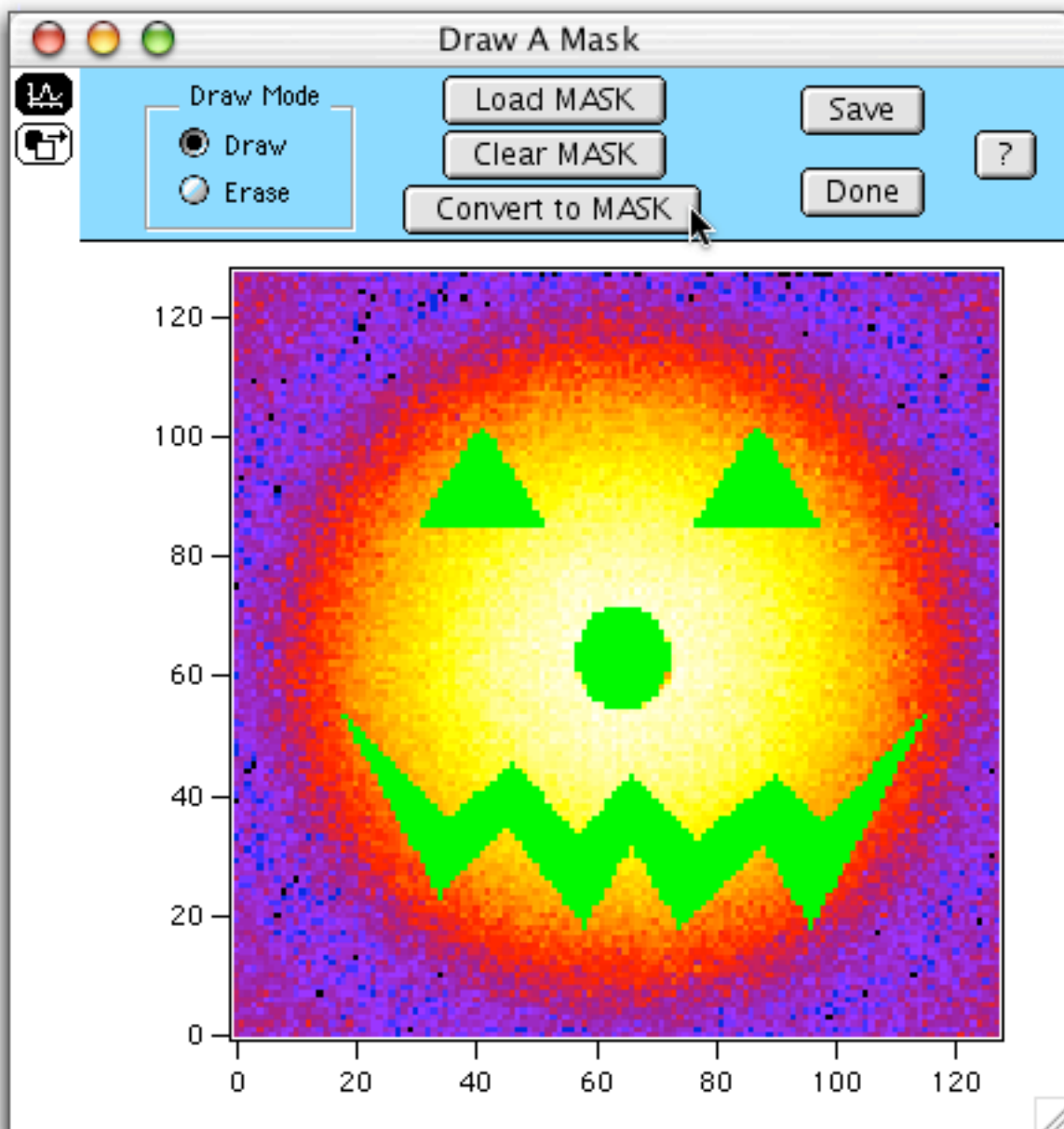
Save: saves the current mask to disk, also copies the saved mask to the MSK folder for immediate use.

Done: closes the window, first prompting you to save your newly drawn mask.

Tools/Graph Toggle: switches between modes where the Tool Bar is visible (below, left) or hidden (below, right). When the Tool Bar is visible, the buttons in the top control bar are inactive. When the Tool Bar is hidden, the control buttons are activated.



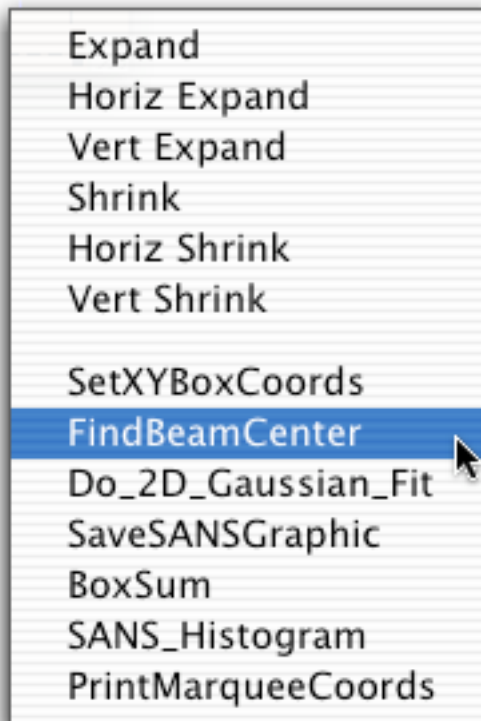
To draw a simple mask, hide the tool bar and set the mode to "Draw" using the radio buttons. Make the tool bar visible again, and select any of the polygon or circle drawing tools. Lines or text drawn will not be added to the mask. Draw the desired objects, and hide the tools. Click "Convert To MASK", and the (white) draw objects will be replaced with a green mask image. Mistakes can be "Erased", or "Clear MASK" will start fresh again. Be sure to save your mask before leaving. Once saved, the mask is pre-loaded, and can be immediately viewed on your data by clicking "Show Mask" in the Display window.



Marquee Operations

What: The marquee menu, invoked from a marquee selection on the SANS Data Display provides several new operations.

How: Click and drag a marquee region in the SANS Data Display window. Then move the cursor inside the selection (to get an upside-down hat cursor) and click to get a new menu like this:



The operations are:

SetXYBoxCoords: is used (only) by the Calculate Transmission operation for setting the box range of the empty beam transmission file.

FindBeamCenter: reports the centroid (intensity-weighted) of the selected region. Results are reported in detector coordinates (1,128) and can be directly used to Patch beamcenter values in raw SANS file headers.

Do_2D_Gaussian_Fit: performs a 2-D Gaussian fit over the selected region. The results for the fit are reported to the command window and displayed as a new contour plot of the fit with an image of the data behind. The details of the coefficients of the 2D Gaussian model can be found in Igor's on-line help files. Note that if the region is sufficiently non-Gaussian, the fit may not converge and report an error.

SaveSANSGraphic: presents Igor's save graphics dialog to allow you to save the 2D image (with the color scale, but not the control bar). The image can be saved in a variety of formats. PNG (2x screen) is a good cross-platform choice with a reasonable (33kB) file size.

BoxSum: takes the selected XY region, then prompts you for a comma-delimited list of file numbers over which you would like to sum the selected region. Each file is then normalized by "adding" to SAM, then the Box Sum for each file is computed and reported to the command window and displayed in a graph of counts versus run number.

SANS_Histogram: generates a histogram of counts vs. pixel location in the selected region. Positive values are displayed in red, negative values in blue. Very useful to check the balance of counts around the beamstop for

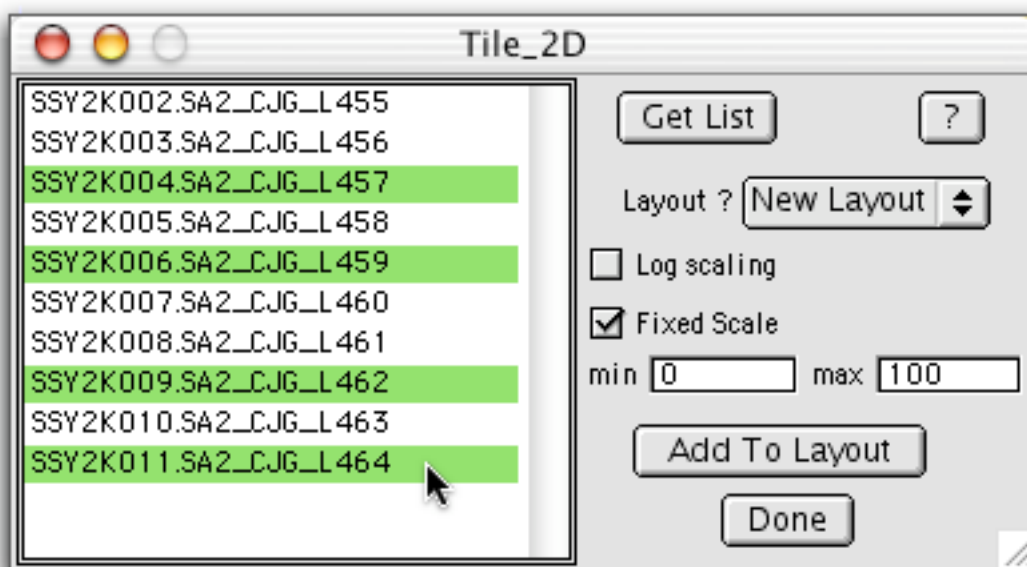
alignment.

PrintMarqueeCoordinates: simply prints the (X,Y) extent of the selection in terms of pixel coordinates.

Tile 2-D Images

What: Allows you to create a layout of small images of a group of raw SANS data files. Often this is useful for viewing systematic trends in sample behavior, for example a sample under an applied shear field.

How: Click the "Tile RAW 2D" button on the 2-D Ops button on the main panel. You will be presented with the following panel:

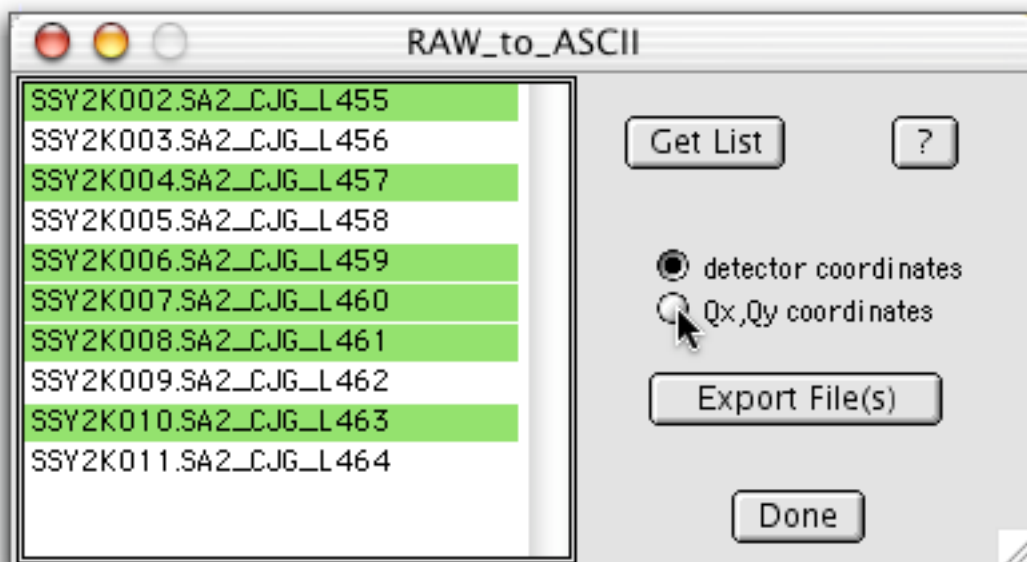


Click "Get List" to see a list of available raw SANS data files. Shift-click to select the desired files. You can choose log or linear scaling of the colors. To better compare a series of data, you can also fix the minimum and maximum values of the color mapping to be the same for all of the selected files. If fixed scale is not selected, each file will be scaled to its own data range. Click "Add To Layout" to append graphics images of each of the selected files to the layout named in the popup list. The images can be arranged as desired, and annotations can be added to the layout using the drawing and text tools. Clicking "Done" will close the panel, first warning that agreeing to close the panel will delete the layouts that you have created and remove the images from memory. There is no harm in keeping the layouts open.

2-D ASCII Export

What: Allows the export of RAW (uncorrected) data files as ASCII text, readable by other graphics packages. Two export types are available, either intensity (neutron counts) versus detector pixel (x,y), or neutron counts versus (Qx,Qy).

How: Open the panel by clicking "RAW ASCII Export" on the Misc Ops tab on the main panel. Click "Get List" to see a list of the raw SANS data files in your data folder. Shift-click to select the files you would like to export. Set the export type using the radio buttons, then click "Export Files" to write the ASCII files to disk. Data files will be automatically named using default names of the form "SSY2K002.ASC".

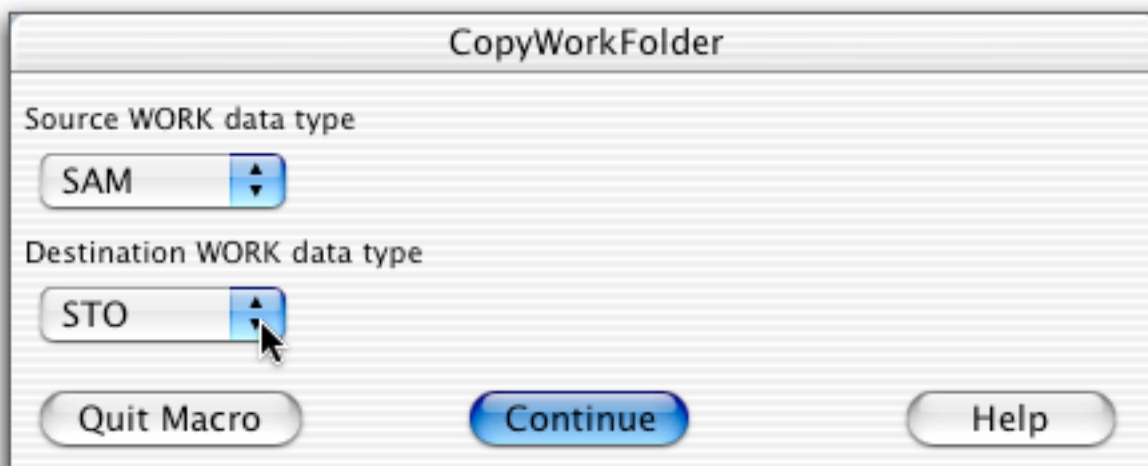


Data exported in detector coordinates is written with a header followed by a single column of data, containing $128 \times 128 = 16384$ elements. Data exported as Qx, Qy coordinates are written as three columns: Qx, Qy, I(Qx,Qy).

Copy Work Folder Contents

What: This operation duplicates the contents of any data folder into another folder. It is often useful to keep a fresh copy of a 2-D dataset when performing math operations on 2-D data.

How: Click the "Copy Work" button on the 2-D Ops button on the main panel. You will be presented with the following dialog, prompting you for the source and destination data folders. Data in the destination folder will be overwritten, and you will not be warned. You can view the new contents of the destination folder by choosing "2D Display" on the same tab of the main panel.

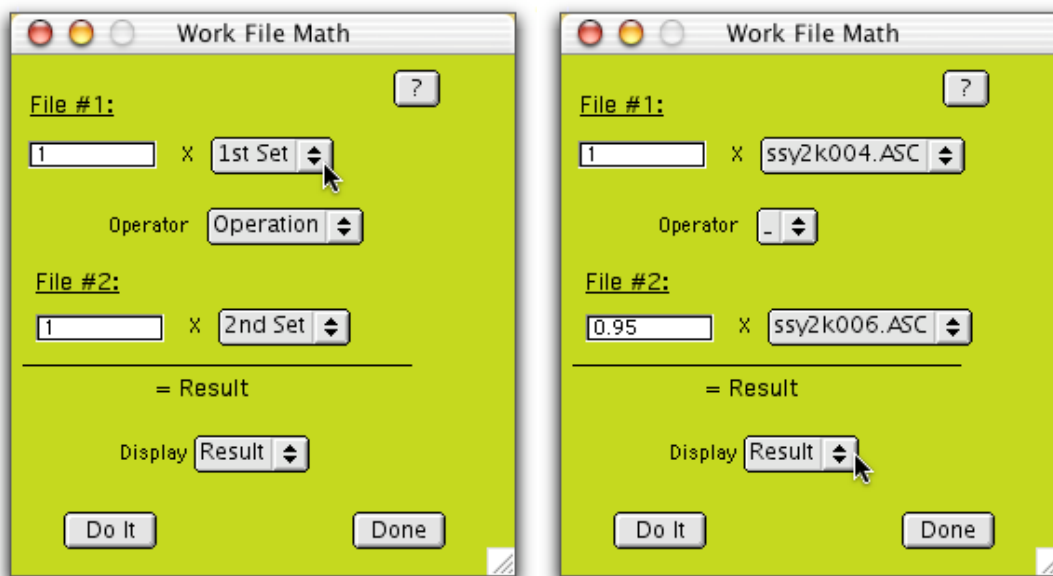


2-D Work File Arithmetic

What: Allows simple arithmetic operations on previously saved 2D ASCII data files, and is particularly useful for fine-tuning background corrections or finding differences in 2-D datasets. Results of the operation are viewed directly, and can be averaged or saved.

How: Click the "WorkFile Math" button on the 2-D Ops button on the Main Panel. You will be presented with the following panel (below, left) prompting you for the operand files, the operation, and the data set to display which is typically the result. Select the appropriate files from the popup menus for the two data files. These files must be 2D ASCII files saved from a reduction protocol, from the Average Panel (see [Average Options](#)), or from Raw [2-D ASCII Export](#). An option for the second operand to be a unit matrix is also available.

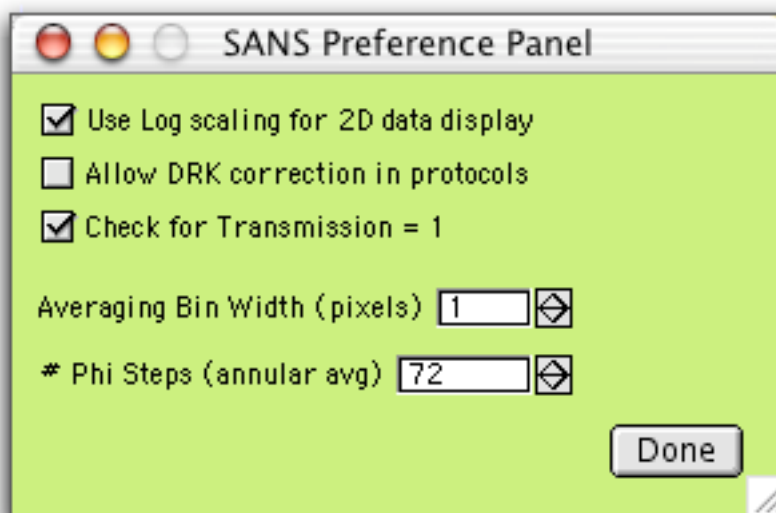
In the example on the right (below), $0.95 \times \text{SSY2K006.ASC}$ will be subtracted from SSY2K004.ASC . The result of the calculation is deposited in a "Result" data set, which will be displayed. The calculation performed will also be echoed to the command window at the bottom of the screen. The result is not automatically saved, but can be averaged or saved as 2D ASCII using the controls on the SANS data display window.



SANS Preferences

What: Set a few display and averaging preferences.

How: From the Misc Ops Tab on the Main Panel, click on "Preferences" to bring up the following panel. The values shown here are the default values. The default values can be reset by selecting "Initialize" from the SANS Menu.



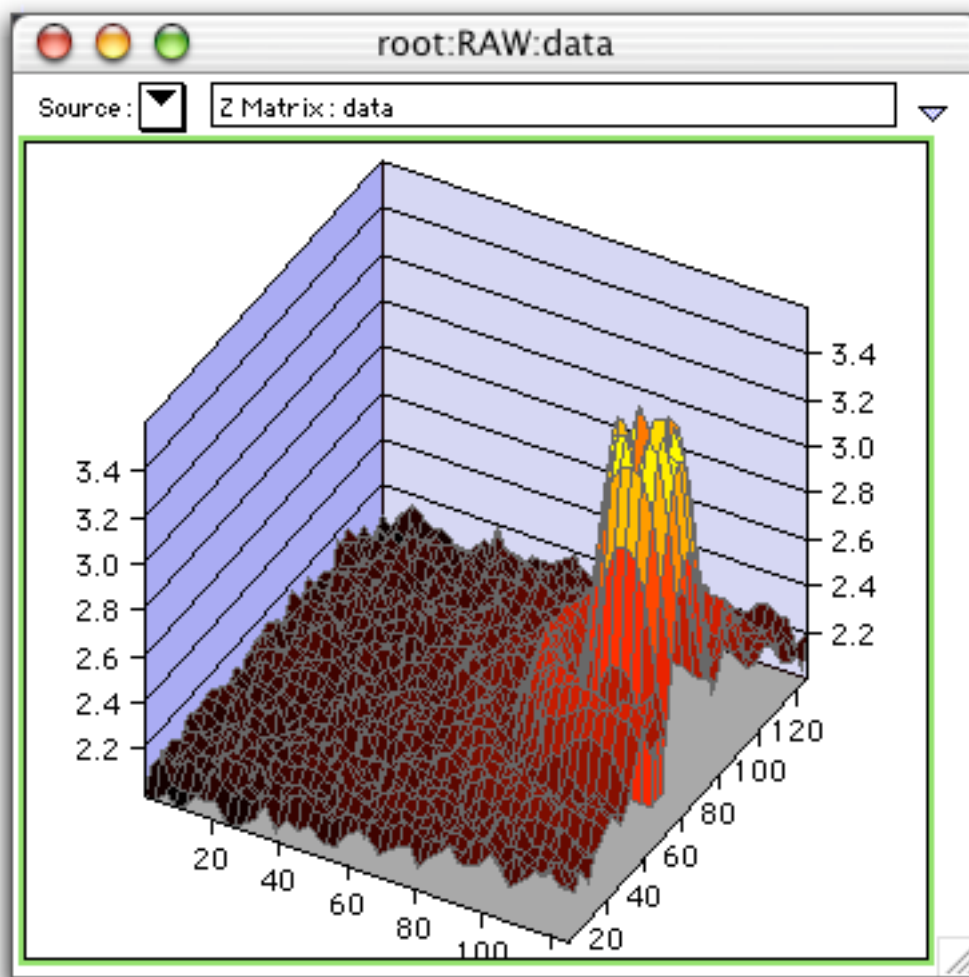
From this panel, you can set:

- the default display for the 2D SANS data, either log or linear scaling of the counts
- allow DRK correction step in data reduction protocols (default is no)
- enable checking for Trans = 1 during data reduction (default is YES do the checking)

- the bin width for 1-D averaging (default is one pixel)
- the number of bins used for an annular average (default is 72)

3-D Display

3-D display of a dataset can be done by clicking "3D Display" on the main panel. Any of the intermediate or raw data files can be displayed, in either log or linear format. To change the scaling, make a 2D display of the same data file, and change its scaling to log or linear as desired - the data in the 3D display will update as well, since it is the same data.

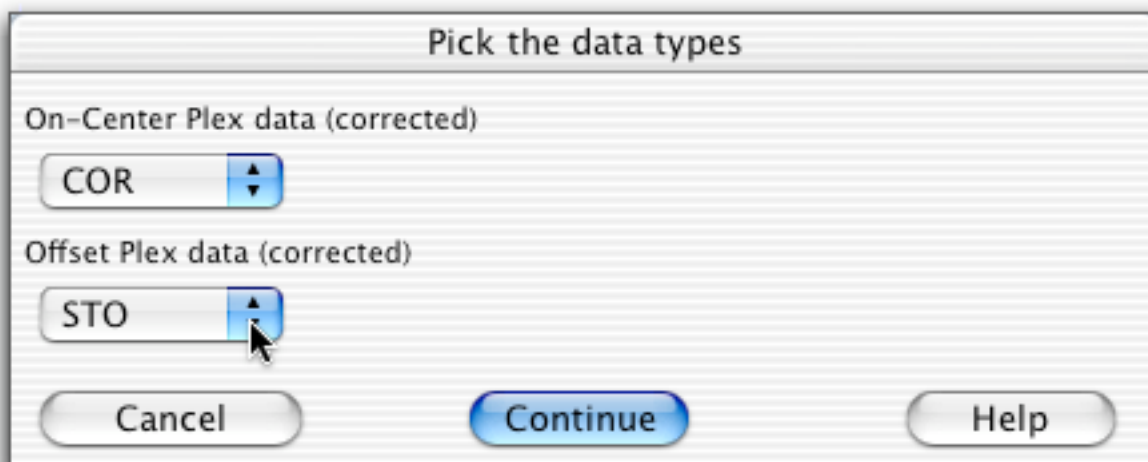


Detector Sensitivity File

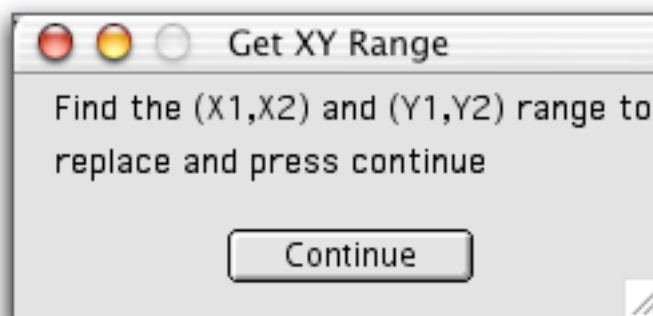
What: Allows a NIST instrument scientist to create a detector sensitivity (DIV) file from within the Igor macros. The work.div file structure created mimics the VAX-generated file and can be used directly in the SANS reduction macros. General users need not perform these steps, as sensitivity files will be provided.

How: At this point, the plexiglass or water files must already be reduced to the COR-level data. In this example, the data with a detector offset was reduced first, then copied into STO,

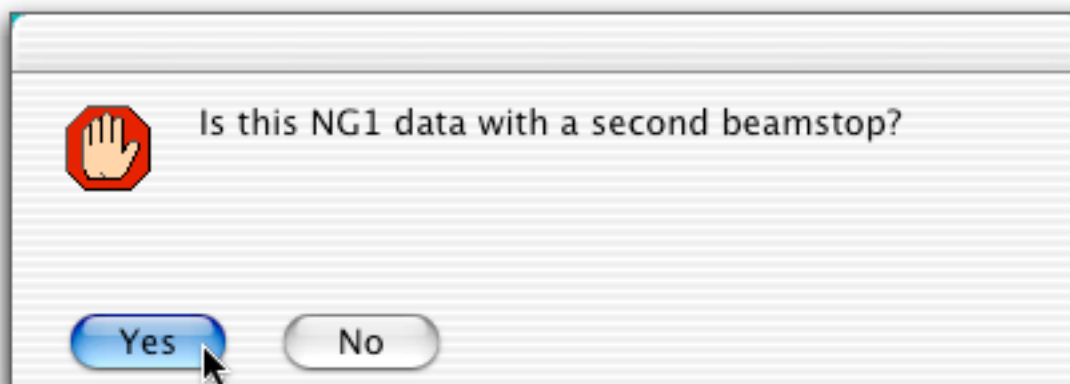
then data with no offset was reduced, ending in COR. Click the "Make DIV File" button on the Misc Ops button on the main panel. You will be presented with the following dialog, prompting you for the "on-center" and "off-center" data folders.



Click "Continue", and the On-center (no offset) data will be displayed. You will be presented with the following instruction panel:



At this point, identify the XY range encompassing the beamstop, the rectangular region that is to be replaced. The region can be identified by simply moving the cursor and noting the pixel values (write them down). If the data is for NG1 where there are two beamstops, write down the XY box for both beamstops. Once you have identified the XY region, click continue, and you will be presented with a simple dialog where you will enter the actual values. The rectangular region of the on-center dataset will be replaced with the same section of the offset data. If the data is for NG1, answer Yes to the following dialog to enter the XY box for the second beamstop - they can be entered in either order. Finally, you will be prompted to save the final, normalized DIV file.



Real Time Data Display

What: Show the live detector image during data collection. Currently this is only in use at the NG1 SANS instrument.

How: From the Raw Data Tab on the main panel, click on "RealTime Display" to bring up the following panel:

A window titled "Real Time Display Controls" with a yellow background. The title bar has standard Mac OS window controls (red, yellow, grey buttons). The text "Enter values for real-time display" is centered at the top. Below this are several input fields and buttons. On the left, there are four input fields: "X Center" with value 64, "Y Center" with value 64, "SDD (m)" with value 5, and "Lambda (A)" with value 6. Below these are "Update Interval (s)" with value 5, "Timeout Interval (s)" with value 300, and "Total Detector Counts" with value 0. On the right side, there are four buttons: "Load Live Data", "Start Updating", "Help", and "Done".

In the fields, enter the approximate beam center, the sample to detector distance, and the wavelength. These parameters are necessary for the calculation of q-values on the data display. Click on "Load Live Data" to load the "live" data set. Check with your local contact for the location and name of this file. Click "Start Updating", to initiate a refresh of the data displayed. In this case, display will be refreshed every 5 seconds (the detector only sends new data on an interval of a few seconds). The refresh will automatically stop after 300 seconds, and the button will revert back to "Start Updating". Since the display automatically re-maps the color scale, the update can be verified by checking the total detector counts, which will increase as data is being collected and the update is active.